

HANDBOOK OF

Computational

Methods for

Integration

Prem K. Kythe
Michael R. Schäferkötter



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To Kiran and Michelle

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Preface

This book started with a simple idea to present in one volume the numerical and computational aspects of integration and quadrature rules, and to include most of the areas where numerical integration is required. This has taken us from quadrature rules for one-dimensional finite and infinite range integrals to their applications in differential and integral equations, Fourier integrals and transforms, Hartley transform, fast Fourier and Hartley transforms, and wavelets.

Since the publication of the book on methods of numerical integration by Davis and Rabinowitz (1984), there has been enormous productivity in theoretical as well as computational integration. Some attempts have been made to find an optimal or the best numerical method and related computer code to put to rest the problem of numerical integration. But the research is continuously ongoing as this problem is still very much open-ended. We have tried to include as much of this research as possible by consulting published research papers and books and citing them.

Some information about the contents of the book is given below. More details can be found in the Table of Contents.

Chapter 1 provides some useful definitions and results on orthogonal polynomials, divided differences, interpolation, convergence acceleration methods, and cubic splines. **Chapter 2** deals with interpolatory quadrature and presents Newton-Cotes rules, Romberg and Gregory integrations, iterative and adaptive schemes, and interpolatory product integration. The Gaussian quadrature and the following rules are discussed in detail in **Chapter 3**: Gauss-Jacobi, Gauss-Legendre, Gauss-Laguerre, Gauss-Hermite, Gauss-Radau, Gauss-Lobatto, Gauss-Chebyshev, Gauss-Log, Clenshaw-Curtis, Gauss-Kronrod, Patterson's, Basu, and Bessel's; Gaussian rules for moments and modified moments are discussed in detail; finite oscillatory

integrals and noninterpolatory product integration are studied. [Chapter 4](#) deals with methods for improper integrals, slowly convergent integrals, infinite-range oscillatory integrals, and product integration. Quadrature rules for singular integrals are presented in [Chapter 5](#); different types of singularities and acceleration techniques are discussed, and Cauchy's p.v. and the Hadamard finite-part integrals are presented. [Chapter 6](#) deals with Fourier integrals and transforms; interpolatory rules for Fourier integrals, rational functions and trigonometric integrals are presented; discrete and fast Fourier transforms, and Hartley and fast Hartley transforms are discussed in detail. [Chapter 7](#) provides a comprehensive account of methods of inversion of the Laplace transform. [Chapter 8](#) deals with wavelets which are presented as an extension of Fourier transform. Although they do not involve numerical integration directly, they are presented to show the advantages they have over traditional Fourier methods in analyzing signals. [Chapter 9](#) covers the areas of Fredholm integral equations of the first and second kind, and singular integral equations.

There are three appendices: [Appendix A](#) contains thirty-two quadrature tables; some simple figures that are mentioned in [Chapters 2, 7, 8 and 9](#) are collectively presented in [Appendix B](#); and the contents of the CD-R which accompanies the book are described in [Appendix C](#).

The CD-R contains tables of over 5800 formulas for indefinite and definite integrals; quadrature tables in ASCII format so they need not be retyped by the users; pdf files listed in [Appendix C](#); and computer codes in C++, f90, MATLAB, and Mathematica, all in ASCII format. This is followed by the [bibliography](#) which is large but by no means complete, and the subject index.

The authors welcome comments and suggestions from readers.

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Notation

A list of the notation, acronyms and abbreviations used in this book is given below.

\arg	argument of a complex number
$(a)_n$	Pochhammer's symbol $= \frac{\Gamma(a+n)}{\Gamma(n)} = a(a+1)\dots(a+n-1)$
$A \times A$	product of sets A and B
$A \setminus B$	complement of a set B with respect to a set A
\bar{A}	closure of a set A
$(Af)(x)$	Lagrangian interpolant [see P_{0,1,...,n}(x)]
$A[a, b]$	class of admissible functions on $[a, b]$
A_k	weights (see w_k)
$A_i(m)$	Lagrangian integration coefficients
A	matrix
A ^T	transpose of a matrix A
$B(m, n)$	beta function $= \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}$
$B_x(p, q)$	incomplete beta function
$B(f)$	Bessel's rule
BR	backward recursion
$B_n, B_{2k}^{(2k)}$	Bernoulli numbers
$B_q(x)$	Bernoulli polynomial of degree q
$C[a, b]$	class of continuous functions on $[a, b]$
$C(x)$	Fresnel cosine integral
$C_\nu(x)$	Young function
C_n^k	Cotesian numbers
$C_n^\mu(x)$	ultraspherical (Gegenbauer) polynomials
$\text{Ci}(x)$	cosine integral

$\chi(x)$	hyperbolic cosine function
CSK1	Cauchy singular equations of the first kind
CSK2	Cauchy singular equations of the second kind
$C^k[a, b]$	class of continuous functions with k continuous derivatives on an interval $[a, b]$
$C^{(k)}(f)$	Fourier (cosine) coefficients
\mathcal{C}	complex plane
$\det(\mathbf{A})$	determinant of a matrix \mathbf{A}
D	domain
DCT	discrete cosine transform
DFT	discrete Fourier transform
DHT	discrete Hartley transform
DST	discrete sine transform
$D_p(z)$	parabolic cylinder functions
\mathbf{D}	Daubechies basis
$\mathbf{e} = \{e_i\}_{i=1}^n$	basis
e.g.	for example
ET	Euler transformation
E_n or $E_n(f)$	error in a rule; also, Euler numbers
Eq(s)	equation(s) (when followed by an equation number)
$E(\varphi, k)$	elliptic integral of the second kind
$\mathbf{E}(k), \mathbf{E}(k')$	complete elliptic integral of the second kind, $k' = \sqrt{1 - k^2}$.
$\mathbf{E}_\nu(z)$	Weber function
$\text{Ei}(x)$	exponential integral function defined by
	$\int_{-\infty}^x \frac{e^t}{t} dt = - \int_{-x}^{\infty} \frac{e^{-t}}{t} dt, \quad x < 0$
$\overline{\text{Ei}(x)}$	= p.v. $\text{Ei}(x)$
$E_m(x)$	exponential integral = $\int_1^{\infty} (e^{-xt}/t^m) dt$
$\text{erf}(x)$	error function
$\text{erfc}(x)$	complementary error function = $1 - \text{erf}(x)$
$f(x)$	free term
$\tilde{f}(s)$	inverse Laplace transform
\tilde{f}	approximation of f
$f^*(z)$	complex conjugate of a function $f(z)$
$f[x_0, \dots, x_n]$	divided difference of linear functions $f(x_0), \dots, f(x_n)$
$F[a, b]$	class of functions in $C[a, b]$ or in $R[a, b]$
$F(\varphi, k)$	elliptic integral of the first kind
${}_2F_1(\alpha, \beta, \gamma; x)$	Gauss hypergeometric function, also $F(\alpha, \beta, \gamma; x)$
$F(\omega)$	Fourier transform of $f(x)$
$F_c(\omega)$	Fourier cosine transform of $f(x)$
$F_s(\omega)$	Fourier sine transform of $f(x)$
FFT	fast Fourier transform
FHT	fast Hartley transform
FK1	Fredholm equation of the first kind

FK2	Fredholm equation of the second kind
FK3	Fredholm equation of the third kind
FLIT	fast inverse Laplace transform
FR	forward recursion
${}_2F_2, {}_3F_2$	hypergeometric functions
${}_nF_m(\cdot, \cdot; x)$	generalized hypergeometric function
F_1, F_2, F_3, F_4	hypergeometric functions of two variables
f	vector
$\mathcal{F}\{f\}$	Fourier transform of $f(t)$ (same as $F(\omega)$)
\mathcal{F}_c	Fourier cosine transform (same as $F_c(\omega)$)
\mathcal{F}_s	Fourier sine transform (same as $F_s(\omega)$)
$F \star G$	type 1 convolution
$F \circ G$	type 2 convolution
$F^{(P)}$	periodized function F with period P
$G_n(f)$	Gaussian rule
GP ³ IR	generalized piecewise polynomial product interpolatory rule
GSJ	generalized smooth Jacobi (weight function)
$G_{p,q}^{m,n} \left(x \left \begin{smallmatrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{smallmatrix} \right. \right)$	Meijer functions
G	Catalan constant ≈ 0.91596559
h	step size
$H(x)$	Heaviside unit step function
$H(\omega)$	Hartley transform
$H_2[\phi]$	Hadamard transform of ϕ
$H_n(x)$	Hermite polynomials of degree n
H^α	Hölder condition for $0 < \alpha \leq 1$
H^1	Lipschitz condition
$H_n(x)$	Hermite polynomial of degree n
$H_\nu^{(1)}(z), H_\nu^{(2)}(z)$	Hankel functions of the first and second kind
$H_n(x)$	Hermite polynomials
$\mathbf{H}_\nu(z)$	Struve functions
$\mathcal{H}^1(R)$	real Hardy space
i.e.	that is
iff	if and only if
I	integral
$I_a^b(f)$	$= \int_a^b f(x) dx$
$I_a^b(wf)$	$= \int_a^b w(x) f(x) dx$
$\tilde{I}(f)$	quadrature rule
I	identity matrix, or operator
$I_n(z)$	modified Bessel functions of the first kind
\Im	imaginary part
IDFT	inverse discrete Fourier transform
IIR	interpolatory integration rule
$\mathbf{J}_\nu(z)$	Anger functions

$J_n(x)$	Bessel function of order n and order zero
$\tilde{J}(f)$	quadrature rule related to Bessel's rule
$k(x, s)$	kernel of an integral equation
$k^*(x, s)$	adjoint (conjugate) kernel
$k^{[n]}(x, s)$	degenerate (separable) kernel
$k_\lambda(x, s)$	resolvent of the kernel $k(x, s)$
$k_n(x, s)$	n -th iterated kernel
$k_\nu(x)$	Bateman function
k^T	transposed kernel
$\mathbf{K}(k), \mathbf{K}(k')$	complete elliptic integral of the first kind, $k' = \sqrt{1 - k^2}$
$K_n(z)$	modified Bessel functions of the second kind
K	integral operator
$l_j(x)$	Lagrange interpolating polynomial
L_1	function space
L_2	function space
L_p	function space, $p \geq 1$
L_n	Lebesgue constant
$L(x)$	Lobachevskiy function
$\mathbf{L}_\nu(z)$	modified Struve function
$\text{li}(x)$	logarithm integral = $\text{Ei}(\ln x)$, $x > 1$
$L_n(x)$	Laguerre polynomials
$L_n^{(\alpha)}(x)$	generalized Laguerre polynomial
$Li_n(z)$	Polylogarithm function of z of order n
\mathcal{L}	Laplace transform $\mathcal{L}\{f(t)\} = \tilde{f}(s)$
\mathcal{L}^{-1}	inverse Laplace transform
LMM	linear multistep method
M_n	modified moments
$M_n(f)$	repeated midpoint rule
M_0, M_1, \dots	starting values of modified moments
$M_0(\alpha, \beta, z)$	(or $M(\alpha, \beta, z)$) Kummer's confluent hypergeometric function
$M_n \sim$	asymptotic expansion of M_n as $n \rightarrow \infty$
$M_{\lambda, \mu}(z)$	Whittaker functions
nS	n significant digits
N_f	number of function evaluations
\mathbf{N}	the set of natural numbers
N-C	Newton-Cotes
$O_n(x)$	Neumann polynomials
p.v., or pv	principal value
$p_i(x)$	polynomials of degree $i = 0, 1, 2, \dots, n$
$\{p_i(x)\}$	set of linearly independent basis functions
PIIR	positive interpolatory (product) integration rule
PIR	product integration rule
$P(a, x)$	incomplete gamma function = $\frac{1}{\Gamma(a)} \int_0^x e^{-t} t^{a-1} dt$

$P_n(x)$	Legendre polynomials of degree n
$P_n^*(x)$	shifted Legendre polynomial
$P_n^{(\alpha)}(x)$	associated Legendre polynomials of the first kind
$P_n^{(\alpha, \beta)}(x)$	Jacobi polynomials of degree n
$P_{0,1,\dots,n}(x)$	Lagrangian interpolant
\mathcal{P}	partition of an interval
\mathcal{P}_n	class of polynomials of degree n
$Q_\nu(z)$	Legendre functions of the second kind
$Q_n(f), Q_n$	quadrature rules $n = 1, 2, \dots, N$
$Q_n^{(0)}(f)$	n -point Gaussian quadrature
$Q_n^{(\alpha)}(x)$	associated Legendre polynomials of the second kind
$R[a, b]$	class of Riemann-integrable functions on $[a, b]$
$R_n(f)$	Riemann sum
$R(f)$	remainder
$\bar{R}(f)$	repeated rectangle rule
RR	recurrence relation
R^n	Euclidean n -space
R^+	set of positive real numbers
$\mathcal{R}(n, m)$	Patterson's rule for $I_a^b(wf)$
\Re	real part
s	variable of the Laplace transform
s_j	quadrature points
$s_{\mu, \nu}(z), S_{\mu, \nu}(z)$	Lommel functions
$S_n(x)$	Schl\"afli polynomials
$S(x)$	Fresnel sine integral
$S_n(x)$	Schl\"afli polynomials
$\text{shi}(x)$	hyperbolic sine integral
$\text{sgn } x$	sign function = $\begin{cases} 1, & x > 0, \\ 0, & x = 0, \\ -1, & x < 0. \end{cases}$
$\text{Si}(x)$	sine integral
s	sample, data
S_n	Riemann sum
$S(f)$	basic Simpson's rule
$S_n(f)$	repeated Simpson's rule
S_k, \bar{S}_k	Sidi's rules
$S^{(k)}(f)$	Fourier (cosine) coefficients
Si	sine integral
SK1	singular equation of the first kind
SK2	singular equation of the second kind
SFK1	singular Fredholm equations of the first kind
SFK2	singular Fredholm equations of the second kind
STFT	short time Fourier transform

$T(f)$	basic trapezoidal rule
$T_n(f)$	repeated trapezoidal rule
$\bar{T}_n(f)$	repeated tangent rule
$T_{n,k}$	n -th trapezoidal rule for 2^k subintervals of $[a, b]$
$T^{[m,1]}$	m -panel trapezoidal rule on $[0, 1]$
$T_n(x)$	Chebyshev polynomials of the first kind of degree n
$T_n^*(x)$	shifted Chebyshev polynomials of the first kind of degree n
$U(t - a)$	unit step function ($= 1$ if $t > a$; $1/2$ if $t = a$; -1 if $t < a$)
$U(\alpha, \beta, z)$	Kummer's confluent hypergeometric function
$U_n(x)$	Chebyshev polynomials of the second kind of degree n
$U_n(w, z)$	Lommel functions of two variables
$V_n(w, z)$	Lommel functions of two variables
v_j	weights in generalized quadrature rules
$V_a^b(f)$	total variation of f over the interval $[a, b]$
$V_k(f)$	quadrature rule
V_n	linear vector space
$W_n(f)$	repeated Weddle's rule
$W(n)$	triangular window function
$W_{\lambda, \mu}(z)$	Whittaker functions
$w(x)$	weight function
w_k	Gaussian weights
$w_{n,k}$	weights
$Wf(a, b)$	wavelet transform
WFT	windowed Fourier transform
$\lfloor x \rfloor$	integral part of a real number x
$x = m(k)n$	values of x from m to n step k
x_i	nodes (abscissae, or quadrature points); Nyström points
$x_{n,k}$	nodes
\mathbf{x}^T	transpose of a matrix \mathbf{x}
\mathcal{X}	Banach space
$Y_n(z)$	Neumann functions
z^*	complex conjugate of z
$\Re\{z\}$	real part of a complex number z
α	frequency ($\omega = 2\pi\alpha$)
$\beta(x)$	$= \int_0^1 \frac{t^{x-1}}{1+t} dt = \frac{1}{2} \left[\psi\left(\frac{x+1}{2}\right) - \psi\left(\frac{x}{2}\right) \right]$
$\gamma(a, x)$	incomplete gamma function $= \int_0^x e^{-t} t^{a-1} dt$
$\Gamma(a, x)$	incomplete gamma function $= \Gamma(a) - \gamma(a, x)$ $= \int_x^\infty e^{-t} t^{a-1} dt$
γ_e	Euler constant $\approx 0.5772156649^*$

*This constant is usually denoted by γ ; but we use γ_e to avoid confusion with other uses of the letter γ .

$\Gamma(x)$	gamma function
δ_{ij}	Kronecker delta ($= 0$ if $i \neq j$; $= 1$ if $i = j$)
$\delta^{(n)}f$	n -th central difference
$\delta_i(I)$	Gregory correction term to repeated trapezoidal rule
Δ	norm (maximum length) of a subinterval
$\Delta^{(n)}f$	n -th finite forward difference
Δx_k	length of the interval $[x_{k-1}, x_k]$
λ	eigenvalue
λ_n	n -th eigenvalue
$\lambda_i^{(n)}$	Christoffel weights
μ	characteristic value ($= 1/\lambda$)
$\nu(x)$	nu function $= \int_0^\infty \frac{x^t dt}{\Gamma(t+1)}$
$\nu(x, \alpha)$	nu-alpha function $= \int_0^\infty \frac{x^{t+\alpha} dt}{\Gamma(t+\alpha+1)}$
$\zeta(u)$	Weierstrass zeta function
$\zeta(z), \zeta(z, q)$	Riemann zeta function
ξ_j	Chebyshev points; also, Gauss points
$\xi_i^{(n)}$	Christoffel nodes
π	an approximate value of π ($= 3.14159$)
$\pi(x)$	polynomial $(x - x_1)(x - x_2) \dots (x - x_n)$
$\Pi(x)$	Lobachevskiy angle of parallelism
$\Pi(\varphi, n, k)$	elliptic integral of the third kind
$\sigma(x)$	Weierstrass sigma function
ϕ	unknown function in an integral equation
$\phi(t)$	scaling function of a wavelet; father wavelet
$\Phi(\omega)$	Fourier transform of $\phi(t)$
$\Phi(z, s, v)$	Lerch function
$\Phi(a, c; x)$	confluent hypergeometric function $= {}_1F_1(\alpha; \gamma; x)$
$\Phi_1(\alpha, \beta, \gamma, x, y)$	degenerate hypergeometric series in two variables
$\psi(x)$	Euler psi function
$\tilde{\phi}$	approximate value of ϕ
$\tilde{\Phi}$	vector of approximate solutions $\tilde{\phi}$'s; also, blocks
$\chi_{[a,b]}(x)$	characteristic function on $[a, b]$
$\psi(x)$	(mother) wavelet
$\Psi(\omega)$	Fourier transform of a wavelet $\psi(t)$
ω	radian frequency ($\omega = 2\pi\alpha$)
$\omega(f, \delta)$	modulus of continuity of f
\emptyset	empty set
$\langle u, v \rangle$	inner product of u and v on $[a, b]$ $\left(= \int_a^b f(x)g(x) dx \right)$
∇^2	Laplacian $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$
$\nabla^{(n)}f$	n -th backward difference

\int

Cauchy principal-value (p.v.) integral

\oint

Hadamard (finite-part) integral

\sum'

summation with the first term halved

\sum''

summation with the first and last terms halved

\sum^*

summation with the last term halved if n is odd

$\|\cdot\|$

norm

$n!!$

double factorial defined in §1.3.4

$\operatorname{cas} \theta$

$=\cos \theta + \sin \theta$

$[x_1, \dots, x_n]^T$

column vector

$\binom{m}{n}$

binomial coefficients $= \frac{m!}{n!(m-n)!}$

■

end of a proof or an example

1

Preliminaries

In this chapter we discuss some basic concepts and present results needed to study the numerical and computational aspects of integration. Proofs of most of the results can be found in standard textbooks on numerical analysis, and real and complex analysis. The notation used in this book, although standard, is presented prior to this chapter.

1.1. Notation and Definitions

Let R^n denote the Euclidean n -space and R^+ the set of nonnegative real numbers. The complement of a set B with respect to a set A is denoted by $A \setminus B$, the product of the sets A and B by $A \times B$, and the closure of a set A by \bar{A} .

A real- or complex-valued function f is said to belong to the class $C^k(D)$ if it is continuous together with its k -th derivatives, in a domain D , $0 \leq k < \infty$. In this case we shall often write that f is a $C^k(D)$ -function or that f is a C^k -function on D , and a C^0 -function is written as a C -function. The functions f in the class $C^k(D)$, for which all k -th derivatives admit continuous continuations in the closure \bar{D} , form the class of functions $C^k(\bar{D})$. The class $C^\infty(D)$ consists of functions f that are infinitely differentiable on D ; i.e., continuous partial derivatives of all orders exist. These classes are linear sets. Thus, every linear combination $\lambda f + \mu g$, where λ and μ are arbitrary complex numbers, also belongs to the respective class.

In the case of a real function f of a single variable, which is integrable in the Riemann sense, suppose that $y = f(x)$ is a bounded function on the finite interval $[a, b]$. Partition this interval into n subintervals by the points $a = x_0 < x_1 < \dots < x_n = b$. Let ξ be any point in the i -th subinterval: $x_{i-1} \leq \xi_i \leq x_i$. Then form the

sum

$$S_n = \sum_{i=1}^n f(\xi_i) (x_i - x_{i-1}). \quad (1.1.1)$$

Such a sum is called a *Riemann sum*. Let $\Delta = \max_i (x_i - x_{i-1})$ denote the maximum length (or norm) of the subintervals, and consider a sequence of sums of type (1.1.1), S_1, S_2, \dots , whose respective norms $\Delta_1, \Delta_2, \dots$ are such that $\lim_{m \rightarrow \infty} \Delta_m = 0$. If, for any sequence of this type and any choice of ξ_i , the sequence $\{S_m\}$ has a common limit S , then $f(x)$ is said to have the *Riemann integral* S over the interval $[a, b]$; i.e., $S = \int_a^b f(x) dx$. A bounded function $f(x)$ is Riemann-integrable iff $f(x)$ is continuous almost everywhere. In particular, if $f(x) \in C[a, b]$, it has a Riemann integral. Also, if $f(x)$ is bounded on $[a, b]$ and continuous except for finitely many points of discontinuity, it is Riemann-integrable.

The Schwarz, Hölder, and Minkowski inequalities are, respectively:

$$\left| \int_a^b f(x) g(x) dx \right| \leq \left(\int_a^b |f(x)|^2 dx \right)^{1/2} \left(\int_a^b |g(x)|^2 dx \right)^{1/2}, \quad (1.1.2)$$

$$\left| \int_a^b f(x) g(x) dx \right| \leq \left(\int_a^b |f(x)|^p dx \right)^{1/p} \left(\int_a^b |g(x)|^q dx \right)^{1/q}, \quad p > 1, \quad (1.1.3)$$

$$\left(\int_a^b |f(x) + g(x)|^p dx \right)^{1/p} \leq \left(\int_a^b |f(x)|^p dx \right)^{1/p} \left(\int_a^b |g(x)|^p dx \right)^{1/p}, \quad p \geq 1, \quad (1.1.4)$$

where $1/p + 1/q = 1$.

Let $T : X \mapsto X$ be a linear operator on the normed space X of dimension n . Let $e = \{e_1, \dots, e_n\}$ be any basis for X and let $T_e = (\alpha_{ij})$ be the matrix representing T with respect to that basis whose elements are kept in the given order. Then the eigenvalues of the matrix T_e are called *eigenvalues of the operator* T_e , and the spectrum and the resolvent set are similarly defined. A basis result is as follows: All matrices representing a given linear operator $T : X \mapsto X$ on a finite-dimensional normed space relative to various bases for X have the same eigenvalues. Other results are: (i) a linear operator on a finite-dimensional complex normed space $X \neq \{0\}$ has at least one eigenvalue; (ii) the eigenvalues of a Hermitian (self-adjoint) matrix A are real, whereas those of a skew-Hermitian matrix are purely imaginary or zero, and those of a unitary matrix have absolute value 1.

The theory of numerical integration uses many results from the theory of orthogonal polynomials, theory of interpolation and of finite and divided differences. It is, therefore, necessary that we introduce these topics before we discuss quadrature rules and their convergence. We will say that $f \in \mathcal{P}_n$ if f is a polynomial of degree n .

Two useful formulas are as follows:

(i) The LEIBNIZ RULE for differentiating an integral with respect to a parameter is

$$\begin{aligned} \frac{\partial}{\partial y} \int_a^b g(t, y) dt &= \int_a^b g_y(t, y) dt, \\ \frac{\partial}{\partial y} \int_{h_1(y)}^{h_2(y)} g(t, y) dt &= \int_{h_1(y)}^{h_2(y)} g_y(t, y) dt + h_2'(y) g(h_2(y), y) \\ &\quad - h_1'(y) g(h_1(y), y). \end{aligned} \quad (1.1.5)$$

For details, see [Williamson, Crowell, and Trotter](#) (1962, p.316).

(ii) The POINCARÉ–BERTRAND FORMULA is

$$\begin{aligned} \frac{1}{i\pi} \oint_{\Gamma} \frac{d\zeta}{\zeta - z} \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{\zeta - \zeta_1} d\zeta_1 &= g(z, z) \\ &\quad + \frac{1}{i\pi} \oint_{\Gamma} d\zeta_1 \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{(\zeta - z)(\zeta - \zeta_1)} d\zeta, \end{aligned} \quad (1.1.6)$$

or, alternatively,

$$\oint_{\Gamma} \frac{d\zeta}{\zeta - z} \cdot \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{\zeta - \zeta_1} d\zeta_1 = \pi^2 g(z, z) + \oint_{\Gamma} d\zeta_1 \cdot \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{(\zeta - z)(\zeta - \zeta_1)} d\zeta, \quad (1.1.7)$$

where the function $g(\zeta, \zeta_1)$ satisfies the Hölder condition with respect to both variables. This formula is useful when changing the order of integration in singular integrals.

1.2. Orthogonal Polynomials

Besides the interpolating polynomials, many orthogonal polynomials are important for quadrature methods. The zeros of these polynomials are usually real, distinct, and contained in a particular interval. As such, these systems of zeros are used as nodes of quadrature rules, which possess additional properties, like that of positivity or minimality of the quadrature error. [Table 1.2.1](#) gives the classical polynomials corresponding to their specific weights and intervals.

A set of polynomials $\{p_i\}$ with degree i and such that $\langle p_i, p_j \rangle = 0$ for $i \neq j$ is called a set of orthogonal polynomials with respect to the inner product $\langle p_i, p_j \rangle$ on a finite or infinite interval $[a, b]$. Let $w(x)$ be an admissible weight function on the interval $[a, b]$. If we orthonormalize the powers $1, x, x^2, \dots$, we obtain a unique set of polynomials $p_n(x)$ of degree n and leading coefficient positive, such that

$$\int_a^b w(x) p_n(x) p_m(x) dx = \delta_{mn} = \begin{cases} 0 & \text{if } m \neq n, \\ 1 & \text{if } m = n, \end{cases} \quad (1.2.1)$$

where δ_{mn} is known as the Kronecker delta.

Table 1.2.1

Name	Symbol	Interval	$w(x)$
Chebyshev*, 1st kind	$T_n(x)$	$[-1, 1]$	$(1 - x^2)^{-1/2}$
Chebyshev, 2nd kind	$U_n(x)$	$[-1, 1]$	$(1 - x^2)^{1/2}$
Ultraspherical (Gegenbauer)	$C_n^\mu(x)$	$[-1, 1]$	$(1 - x^2)^{\mu-1/2}, \mu > -1/2$
Hermite	$H_n(x)$	$(-\infty, \infty)$	e^{-x^2}
Jacobi	$P_n^{(\alpha, \beta)}(x)$	$[-1, 1]$	$(1 - x)^\alpha (1 + x)^\beta, \alpha, \beta > -1$
Laguerre	$L_n(x)$	$[0, \infty)$	e^{-x}
Generalized Laguerre	$L_n^\alpha(x)$	$[0, \infty)$	$x^\alpha e^{-x}, \alpha > -1$
Legendre	$P_n(x)$	$[-1, 1]$	1

* Also spelled ‘Tschebyscheff’.

Orthogonal polynomials with respect to the above inner product satisfy another type of orthogonality, known as “discrete” orthogonality. Let \mathcal{P}_n denote the class of all polynomials $p_i(x), i = 1, \dots, n+1$, such that

$$p_n(x_i) = \alpha_i, \quad i = 1, \dots, n+1, \quad (1.2.2)$$

where $x_1 < x_2 < \dots < x_{n+1}$ are $(n+1)$ distinct points and $\alpha_1, \dots, \alpha_{n+1}$ arbitrary numbers.

Let $p_0(x), p_1(x), \dots, p_n(x), p_{n+1}(x)$ be orthonormal polynomials with the weight function $w(x)$ on $[a, b]$. Let x_1, \dots, x_{n+1} be $(n+1)$ zeros of $p_{n+1}(x)$ and let w_1, \dots, w_{n+1} be the respective Gaussian weights. Then

$$\int_a^b w(x) f(x) dx = \sum_{i=1}^{n+1} w_i f(x_i) \quad (1.2.3)$$

for all $f \in \mathcal{P}_{2n+1}$. Now, since $p_j(x)p_k(x) \in \mathcal{P}_{2n+1}$ for $j, k \leq n$, we have

$$\sum_{i=1}^{n+1} w_i p_j(x_i) p_k(x_i) = \int_a^b w(x) p_j(x) p_k(x) dx = \delta_{jk}. \quad (1.2.4)$$

Thus, p_0, p_1, \dots, p_n are orthonormal on the zeros of p_{n+1} with respect to the inner product (1.2.1). Also, if $p_0(x), p_1(x), \dots$ are orthonormal polynomials with $p_n(x) = c_n x^n + \dots, c_n > 0$, with respect to this inner product, then we have the recurrence relation

$$p_{n+1}(x) = (\gamma_n x - a_{nn}) p_n(x) - a_{n,n-1} p_{n-1}(x) - \dots - a_{n0} p_0(x), \quad (1.2.5)$$

for $n = 0, 1, \dots$, where

$$p_0(x) \equiv c_0, \quad \gamma_n = \frac{c_{n+1}}{c_n},$$

$$a_{nk} = \frac{\gamma_n \langle xp_n, p_k \rangle}{\langle p_k, p_k \rangle}, \quad k = 0, 1, \dots, n.$$

Moreover, if the above inner product satisfies the further condition $\langle xp_i, p_j \rangle = \langle p_i, xp_j \rangle$, then the recurrence relation (1.2.5) reduces to the three-term recurrence relation

$$p_{n+1}(x) = (\gamma_n x - \alpha_n) p_n(x) - \beta_n p_{n-1}(x), \quad n = 0, 1, \dots, \quad (1.2.6)$$

where we take $p_{-1}(x) = 0$, and

$$\alpha_n = \frac{\gamma_n \langle xp_n, p_n \rangle}{\langle p_n, p_n \rangle}, \quad n = 0, 1, \dots,$$

$$\beta_n = \frac{\gamma_n \langle xp_n, p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle} = \frac{\gamma_n}{\gamma_{n-1}} \frac{\langle p_n, p_n \rangle}{\langle p_{n-1}, p_{n-1} \rangle}, \quad n = 1, 2, \dots$$

The three-term recurrence relation for $p_n(x)$ yields a “backward” recurrence for an efficient computation of a series expansion of the form $f(x) = \sum_{k=0}^N c_k p_k(x)$. If we set

$$B_k = \begin{cases} 0 & \text{for } k > n, \\ c_k + (\gamma_{k+1}x - \alpha_{k+1}) B_{k+1} - \beta_{k+2} B_{k+2} & \text{for } 0 \leq k \leq n, \end{cases} \quad (1.2.7)$$

then

$$f(x) = \gamma_0 B_0. \quad (1.2.8)$$

Finally, orthogonal polynomials satisfy the Christoffel-Darboux identity

$$\sum_{k=0}^n \frac{p_k(x)p_k(y)}{h_k} = \frac{p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)}{\gamma_n h_n(x-y)}, \quad (1.2.9)$$

where $h_k = \langle p_k, p_k \rangle$. The zeros of some orthogonal polynomials are used in quadrature rules. We consider some of the most frequently used polynomials. Information on others is available in Abramowitz and Stegun (1968).

1.2.1. Chebyshev Polynomials of the First Kind $T_n(x) = \cos(n \arccos x)$, $n = 0, 1, \dots$, over the interval $[-1, 1]$, such that $T_n(1) = 1$. The m -th zero $x_{n,m}$ of $T_n(x)$ is given by

$$x_{n,m} = \cos \frac{(2m-1)\pi}{2n}.$$

It satisfies the orthogonality condition

$$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} T_n(x) T_m(x) dx = \begin{cases} 0 & \text{if } n \neq m, \\ \pi/2 & \text{if } n = m \neq 0, \\ \pi & \text{if } n = m = 0. \end{cases}$$

The three-term recurrence relation is $T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x)$. Other relevant data are as follows:

Norm: $\int_{-1}^1 (1-x^2)^{-1/2} [T_n(x)]^2 dx = \begin{cases} \frac{\pi}{2}, & n \neq 0, \\ \pi, & n = 0; \end{cases}$

Series form: $T_n(x) = \frac{n}{2} \sum_{k=0}^{[n/2]} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!} (2x)^{n-2k} = \cos(n \arccos x);$

Indefinite and definite integrals: $\int T_0 dx = T_1, \int T_1 dx = \frac{T_2}{4},$
 $\int T_n dx = \frac{1}{2} \left[\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1} \right], \quad \int_{-1}^1 T_n dx = \begin{cases} \frac{2}{1-n^2}, & n \text{ even}, \\ 0, & n \text{ odd}; \end{cases}$

Inequality: $|T_n(x)| \leq 1, \quad -1 \leq x \leq 1;$

Rodrigues' formula: $T_n(x) = \frac{(-1)^n (1-x^2)^{1/2} \sqrt{\pi}}{2^{n+1} \Gamma(n+1/2)} \frac{d^n}{dx^n} \{(1-x^2)^{n-1/2}\}.$

A useful formula which is a special case of the Christoffel-Darboux formula (see [Davis 1976](#)) is

$$\frac{1}{2} [T_{n+1}(x) T_n(y) - T_{n+1}(y) T_n(x)] = (x-y) \sum_{k=0}^n {}' T_k(x) T_k(y). \tag{1.2.10}$$

Table 1.2.2. Coefficient Triangle.

	x^0	x^1	x^2	x^3	x^4	x^5	x^6	x^7	x^8	x^9	x^{10}
$T_0(x)$	1										
$T_1(x)$		1									
$T_2(x)$	-1		2								
$T_3(x)$		-3		4							
$T_4(x)$	1		-8		8						
$T_5(x)$		5		-20		16					
$T_6(x)$	-1		18		-48		32				
$T_7(x)$		-7		56		-112		64			
$T_8(x)$	1		-32		160		-256		128		
$T_9(x)$		9		-120		432		-576		256	
$T_{10}(x)$	-1		50		-400		1120		-1280		512

The coefficients $D_{n,m}$ of x^m in $T_n(x)$ are calculated by the recurrence relation

$$D_{n,m} = 2D_{n-1,m-1} - D_{n-2,m}, \quad n \geq 2, \quad m < n, \quad (1.2.11)$$

which yields the ‘coefficient triangle’ presented in Table 1.2.2, e.g., for $T_n(x)$, $n = 0, 1, \dots, 10$ (the blank represents zero).

1.2.2. Chebyshev Polynomials of the Second Kind $U_n(x)$ over the interval $[-1, 1]$, such that $U_n(1) = n + 1$. The m -th zero $x_{n,m}$ of $U_n(x)$ is given by

$$x_{n,m} = \cos \frac{m\pi}{n+1}.$$

It satisfies the orthogonality condition

$$\int_{-1}^1 \sqrt{1-x^2} U_n(x) U_m(x) dx = \begin{cases} 0 & \text{if } n \neq m, \\ \pi/2 & \text{if } n = m \neq 0, \\ \pi & \text{if } n = m = 0. \end{cases}$$

The three-term recurrence relation is $U_{n+1}(x) = 2x U_n(x) - U_{n-1}(x)$. Other relevant data include:

$$\text{Norm: } \int_{-1}^1 (1-x^2)^{1/2} [U_n(x)]^2 dx = \frac{\pi}{2};$$

$$\text{Series form: } U_n(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{(n-k)!}{k!(n-2k)!} (2x)^{n-2k} = \frac{T'_{n+1}(x)}{n+1},$$

$$U_n(\cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta};$$

$$\text{Definite integral: } \int_{-1}^1 U_n dx = \begin{cases} \frac{2}{n+1}, & n = 2m, \\ 0, & n = 2m+1; \end{cases}$$

$$\text{Inequality: } |U_n(x)| \leq n+1, \quad -1 \leq x \leq 1;$$

$$\text{Rodrigues' formula: } U_n(x) = \frac{(-1)^n (n+1) \sqrt{\pi}}{(1-x^2)^{1/2} 2^{n+1} \Gamma(n+3/2)} \frac{d^n}{dx^n} \{(1-x^2)^{n+1/2}\}.$$

1.2.3. Gegenbauer (or Ultraspherical) Polynomials $C_n^\mu(x)$ over the interval $[-1, 1]$ such that $C_n^\mu(1) = \binom{n+2\mu-1}{n}$. Other relevant data are:

$$\text{Norm: } \int_{-1}^1 (1-x^2)^{\mu-1/2} [C_n^\mu(x)]^2 dx = \frac{\pi 2^{1-2\mu} \Gamma(n+2\mu)}{n! (n+\mu) [\Gamma(\mu)]^2}$$

$$\text{Series form: } C_n^\mu(x) = \frac{1}{\Gamma(\mu)} \sum_{k=0}^{[n/2]} (-1)^k \frac{\Gamma(\mu+n-k)!}{k!(n-2k)!} (2x)^{n-2k};$$

$$\text{Inequality: } \max_{-1 \leq x \leq 1} |C_n^\mu(x)| = \begin{cases} \binom{n+2\mu-1}{n}, & \text{if } \mu > 0, \\ |C_n^\mu(x')|, & \text{if } -1/2 < \mu < 0, \end{cases}$$

where $x' = 0$ if $n = 2k$; $x' = \text{maximum point nearest zero}$ if $n = 2k + 1$;

$$\begin{aligned} \text{Rodrigues' formula: } C_n^\mu(x) &= \frac{(-1)^n 2^n n! \Gamma(\mu + n + 1/2)}{\Gamma(\mu + 1/2) \Gamma(n + 2\mu) (1 - x^2)^{\mu-1/2}} \\ &\quad \times \frac{d^n}{dx^n} \{(1 - x^2)^{n+\mu-1/2}\}. \end{aligned}$$

1.2.4. Hermite Polynomials $H_n^{(\alpha)}(x)$ over the interval $(-\infty, \infty)$, such that

$$\text{Norm: } \int_{-\infty}^{\infty} e^{-x^2} [H_n^{(\alpha)}(x)]^2 dx = \sqrt{\pi} 2^n n!;$$

$$\begin{aligned} \text{Inequality: } |H_{2n}(x)| &\leq e^{x^2/2} 2^{2n} n! \left[2 - \frac{1}{2^{2n}} \binom{2n}{n} \right], \\ |H_{2n+1}(x)| &\leq |x| e^{x^2/2} \frac{(2n+2)!}{(n+1)!}; \end{aligned}$$

$$\text{Rodrigues' formula: } H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

The three-term recurrence relation is $H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x)$.

1.2.5. Jacobi Polynomials $P_n^{(\alpha, \beta)}(x)$ over the interval $[-1, 1]$, such that $P_n^{(\alpha, \beta)}(1) = \binom{n+\alpha}{n}$. Other relevant data are:

$$\begin{aligned} \text{Norm: } \int_{-1}^1 (1-x)^\alpha (1+x)^\beta [P_n^{(\alpha, \beta)}(x)]^2 dx \\ = \frac{2^{\alpha+\beta+1} \Gamma(n+\alpha+1) \Gamma(n+\beta+1)}{(2n+\alpha+\beta) n! \Gamma(n+\alpha+\beta+1)}; \end{aligned}$$

$$\text{Series form: } P_n^{(\alpha, \beta)}(x) = \frac{1}{2^n} \sum_{k=0}^{[n/2]} \binom{n+\alpha}{k} \binom{n+\beta}{n-k} (x-1)^{n-k} (x+1)^k;$$

$$\text{Inequality: } \max_{-1 \leq x \leq 1} |P_n^{(\alpha, \beta)}(x)| = \begin{cases} \binom{n+q}{n} \sim n^q & \text{if } q = \max(\alpha, \beta) \geq -1/2, \\ |P_n^{(\alpha, \beta)}(x')| \sim n^{-1/2} & \text{if } q < -1/2, \end{cases}$$

where x' is one of the two maximum points nearest $(\beta - \alpha)/(\alpha + \beta + 1)$;

$$\begin{aligned} \text{Rodrigues' formula: } P_n^{(\alpha, \beta)}(x) &= \frac{(-1)^n}{2^n n! (1-x)^\alpha (1+x)^\beta} \\ &\quad \times \frac{d^n}{dx^n} \{(1-x)^{n+\alpha} (1+x)^{n+\beta}\}. \end{aligned}$$

1.2.6. Laguerre Polynomials $L_n(x)$ over the interval $[0, \infty)$, such that $L_n(0) = n!$ and

$$\int_0^\infty e^{-x} L_n(x) L_m(x) dx = \begin{cases} 0 & \text{if } n \neq m, \\ (n!)^2 & \text{if } n = m. \end{cases}$$

Its m -th zero $x_{n,m}$ is given by

$$x_{n,m} = \frac{j_m^2}{4k_n} \left(1 + \frac{j_m^2 - 2}{48k_n^2} \right) + O(n^{-5}),$$

where $k_n = n+1/2$ and j_m is the m -th positive zero of the Bessel function $J_n(x)$. The three-term recurrence relation is $(n+1)L_{n+1}(x) = [(2n+1)-x]L_n(x) - nL_{n-1}(x)$. Other relevant data are

Norm: $\int_0^\infty e^{-x} [L_n(x)]^2 dx = 1;$

Series form: $L_n(x) = \sum_{k=0}^n (-1)^k \binom{n}{n-k} \frac{1}{k!} x^k;$

Inequality: $|L_n(x)| = \begin{cases} e^{x/2}, & \text{if } x \geq 0, \\ \left[2 - \frac{1}{n!} \right] e^{x/2}, & \text{if } x \leq 0; \end{cases}$

Rodrigues' formula: $L_n(x) = \frac{1}{n!e^{-x}} \frac{d^n}{dx^n} \{x^n e^{-x}\}.$

1.2.7. Generalized Laguerre Polynomials $L_n^\alpha(x)$ over the interval $[0, \infty)$, such that its m -th zero $x_{n,m}$ is given by

$$x_{n,m} = \frac{j_{\alpha,\beta}^2}{4k_n} \left(1 + \frac{2(\alpha^2 - 1) + j_{\alpha,m}^2}{48k_n^2} \right) + O(n^{-5}),$$

where $k_n = n + (\alpha + 1)/2$, $\alpha > -1$, and $j_{\alpha,m}$ is the m -th positive zero of the Bessel function $J_n(x)$. Other relevant data are

Norm: $\int_0^\infty x^\alpha e^{-x} [L_n^\alpha(x)]^2 dx = \frac{\Gamma(n + \alpha + 1)}{n!};$

Series form: $L_n^\alpha(x) = \sum_{k=0}^n (-1)^k \binom{n + \alpha}{n - k} \frac{1}{k!} x^k;$

Inequality: $|L_n^\alpha(x)| = \begin{cases} \frac{\Gamma(n + \alpha + 1)}{n! \Gamma(\alpha + 1)} e^{x/2}, & \text{if } x \geq 0, \alpha \geq 0, \\ \left[2 - \frac{\Gamma(n + \alpha + 1)}{n! \Gamma(n + 1)} \right] e^{x/2}, & \text{if } x \geq 0, -1 < \alpha < 0; \end{cases}$

Rodrigues' formula: $L_n^\alpha(x) = \frac{1}{n!x^\alpha e^{-x}} \frac{d^n}{dx^n} \{x^{n+\alpha} e^{-x}\}.$

1.2.8. Legendre Polynomials $P_n(x)$ over the interval $[-1, 1]$, such that $P_n(1) = 1$. If $x_{n,m}$ denotes the m -th zero of $P_n(x)$, where $x_{n,1} > x_{n,2} > \cdots > x_{n,n}$, then

$$x_{n,m} = \left(1 - \frac{1}{8n^2} + \frac{1}{8n^3}\right) \cos \frac{(4m-1)\pi}{4n+2} + O(n^{-4}).$$

The three-term recurrence relation is $(n+1)P_{n+1}(x) = (2n+1)xL_n(x) - nL_{n-1}(x)$. Other relevant data are:

$$\text{Norm: } \int_{-1}^1 [P_n(x)]^2 dx = \frac{2}{2n+1};$$

$$\text{Series form: } P_n(x) = \frac{1}{2^n} \sum_{k=0}^{[n/2]} (-1)^k \binom{n}{k} \binom{2n-2k}{n} x^{n-2k};$$

$$\text{Indefinite Integral: } \int P_n(x) dx = \frac{1}{2n+1} [P_{n+1}(x) - P_{n-1}(x)];$$

$$\text{Inequality: } |P_n(x)| \leq 1, \quad -1 \leq x \leq 1;$$

$$\text{Rodrigues' formula: } P_n(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} \{(1-x^2)^n\}.$$

The orthonormal Legendre polynomials $p_n(x)$ are defined by

$$p_n(x) = \sqrt{\frac{2n+1}{2}} P_n(x),$$

with the leading coefficient of $p_n(x)$ is

$$a_n = \sqrt{\frac{2n+1}{2}} \frac{(2n)!}{2^n (n!)^2}.$$

There are some other polynomials that arise in quadrature and have weights $w(x) = \ln x$ on $[0, 1]$, $w(x) = \sin x$ on $[0, \pi]$, and $w(x) = \cos x$ on $[-\pi/2, \pi/2]$.

1.2.9. Shifted Legendre Polynomials. These polynomials, denoted by $P_n^*(x)$, are defined on the interval $0 \leq x \leq 1$. They are obtained from the Legendre polynomials $P_n(x)$, which are defined in $[-1, 1]$, by substituting $2x - 1$ for x in $P_n(x)$. They are defined by

$$P_n^*(x) = (-1)^n \sum_{k=0}^n (-1)^k \binom{n}{k} \frac{(n+k)!}{n! k!} x^k. \quad (3.1.12)$$

A few shifted Legendre polynomials are

$$\begin{aligned}
 P_0^*(x) &= 1, \\
 P_1^*(x) &= 2x - 1, \\
 P_2^*(x) &= 6x^2 - 6x + 1, \\
 P_3^*(x) &= 20x^3 - 30x^2 + 12x - 1, \\
 P_4^*(x) &= 70x^4 - 140x^3 + 90x^2 - 20x + 1, \\
 P_5^*(x) &= 252x^5 - 630x^4 + 560x^3 - 210x^2 + 30x - 1.
 \end{aligned}$$

The shifted Legendre polynomials $P_n^*(x)$ have the additional advantage that its coefficients are all integers, and they satisfy the normality condition

$$\int_0^1 |P_n^*(x)|^2 dx = \frac{1}{2n+1}.$$

Since the polynomials $P_n^*(x)$ are orthogonal, any well-behaved function $f(x)$ can be expanded into a series of the shifted Legendre polynomials. Thus,

$$f(x) = \sum_{n=0}^{\infty} A_n P_n^*(x),$$

where $A_n = (2n+1) \int_0^1 f(x) P_n^*(x) dx$.

EXAMPLE 1.2.1. Zeros of the Legendre polynomial of degree 9 are $x_1 = -0.96816$, $x_2 = -0.836031$, $x_3 = -0.613372$, $x_4 = -0.324253$, $x_5 = 0$, $x_6 = 0.324253$, $x_7 = 0.613372$, $x_8 = 0.836031$, $x_9 = 0.96816$.

Zeros of the shifted Legendre polynomial of degree 9 are

$$y_1 = 0.01592, y_2 = 0.081984, y_3 = 0.193314, y_4 = 0.337874, y_5 = 0.5, \\ y_6 = 0.662127, y_7 = 0.806686, y_8 = 0.918016, y_9 = 0.98408.$$

Some of the weights w'_j corresponding to the shifted Legendre polynomials are $w'_1 = w'_9 = 0.040637$, $w'_2 = w'_8 = 0.090325$, $w'_3 = w'_7 = 0.13030$, $w'_4 = w'_6 = 0.15617$, $w'_5 = 0.16512$. ■

1.2.10. Shifted Chebyshev Polynomials. The *shifted Chebyshev polynomials*, denoted by $T^*(x)$ and $U^*(x)$, respectively, are defined in the same manner as the shifted Legendre polynomials, by replacing x in $T_n(x)$ or $U_n(x)$ by $2x - 1$. Some of the shifted Chebyshev polynomials are

$$\begin{aligned}
 T_0^*(x) &= 1, & U_0^*(x) &= 1, \\
 T_1^*(x) &= 2x - 1, & U_1^*(x) &= 4x - 2, \\
 T_2^*(x) &= 8x^2 - 8x + 1, & U_2^*(x) &= 16x^2 - 16x + 3, \\
 T_3^*(x) &= 32x^3 - 48x^2 + 18x - 1, & U_3^*(x) &= 64x^3 - 96x^2 + 40x - 4.
 \end{aligned}$$

In general,

$$T_n^*(x) = (-1)^n \sum_{k=0}^n (-1)^k \binom{n}{k} 2^k \frac{n(n+1) \dots (n-k+1)}{(2k-1)!!} x^k, \quad (1.2.13a)$$

$$U_n^*(x) = \frac{(-1)^n 2^n (2n+1)!!}{(n+2)(n+3) \dots (2n+1)} \sum_{k=0}^n (-1)^k \binom{n}{k} 2^k \frac{(n+2) \dots (n+k+1)}{(2k-1)!!} x^k, \quad (1.2.13b)$$

or, in terms of the trigonometric notation,

$$T_n^*(x) = \cos(n \arccos(2x-1)), \quad (1.2.14a)$$

$$U_n^*(x) = \frac{\sin((n+1) \arccos(2x-1))}{2\sqrt{x(1-x)}}. \quad (1.2.14b)$$

The double factorial used in the above formulas is defined as follows (Abramowitz and Stegun 1968, p. 258):

$$(2n)!! = 2 \cdot 4 \cdot 6 \dots (2n) = 2^n n!,$$

$$(2n-1)!! = 1 \cdot 3 \cdot 5 \dots (2n-1) = \pi^{-1/2} 2^n \Gamma(n + \frac{1}{2}).$$

1.2.11. Shifted Jacobi Polynomials. The Jacobi polynomials $P_n^{(\alpha, \beta)}(x)$ reduce to the Legendre polynomials $P_n(x)$ for $\alpha = \beta = 0$, and to the Chebyshev polynomials $T_n(x)$ and $U_n(x)$ for $\alpha = \beta = \pm 1/2$, respectively. Generally, for $\alpha = \beta$ the Jacobi polynomials are known as *ultraspherical* or *Gegenbauer polynomials*. The Jacobi polynomials satisfy the recurrence relations

$$\begin{aligned} P_{n+1}^{(\alpha, \beta)}(x) \\ = \frac{\gamma[\alpha^2 - \beta^2 + (\gamma^2 - 1)x]P_n^{(\alpha, \beta)}(x) - 2(n+\alpha)(n+\beta)(\gamma+1)P_{n-1}^{(\alpha, \beta)}(x)}{2(n+1)(\gamma-n)(\gamma-1)}, \end{aligned} \quad (1.2.15)$$

with $\gamma = 2n + \alpha + \beta - 1$, and the initial values are $P_0^{(\alpha, \beta)}(x) = 1$, $P_1^{(\alpha, \beta)}(x) = \frac{1+\alpha}{2}(x+1) + \frac{1+\beta}{2}(x-1)$. These three-term recurrence relations are very useful in computation.

The shifted Jacobi polynomials $P_n^{*(\alpha, \beta)}(x)$ are defined on the interval $[-1, 1]$. They are related to the Jacobi polynomials, which are defined on the interval $[0, 1]$, by $P_n^{*(\alpha, \beta)}(x) = P_n^{(\alpha, \beta)}(2x-1)$, and defined by

$$P_n^{*(\alpha, \beta)}(x) = \frac{(-1)^n}{n} x^{-\alpha} (1-x)^{-\beta} \frac{d^n}{dx^n} [x^{\alpha+n} (1-x)^{\beta+n}], \quad (1.2.16)$$

which is sometimes called Rodrigues' formula for $P_n^{*(\alpha, \beta)}(x)$.

The Jacobi polynomials and the Chebyshev polynomials are related by

$$P_n^{(-1/2, -1/2)}(x) = b_n T_n(x), \quad \text{where } b_n = \frac{\Gamma(2n)}{2^{2n-1} \Gamma(n+1)}, \quad (1.2.17a)$$

$$P_n^{(1/2, 1/2)}(x) = c_n U_n(x), \quad \text{where } c_n = \frac{(2n+1)!}{2^{2n} n! (n+1)!}; \quad (1.2.17b)$$

$$P_n^{*(-1/2, -1/2)}(x) = b_n T_n^*(x), \quad (1.2.18a)$$

$$P_n^{*(1/2, 1/2)}(x) = c_n U_n^*(x). \quad (1.2.18b)$$

Finally, for any polynomial $p(x) \in \mathcal{P}_n$, which has the leading coefficient equal to unity, i.e., $p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_0$, the following result holds (Krylov and Skoblya 1977):

$$\int_{-1}^1 |p(x)| dx \geq 2^{-n+1},$$

where the equality is true only for $p(x) = 2^{-n} U_n(x)$.

1.3. Finite and Divided Differences

We will discuss the finite and divided differences, which will be useful in deriving quadrature formulas.

1.3.1. Finite Differences. Suppose that the values of a function $f(x)$ are known at the equally-spaced points $x_k = x_0 + kh$, $k = 0, 1, 2, \dots$, and let us use the notation: $f_0 = f(x_0)$, $f_1 = f(x_1)$, \dots , $f_k = f(x_k)$. Then the quantities

$$\Delta f_0 = f_1 - f_0, \quad \Delta f_1 = f_2 - f_1, \dots, \Delta f_n = f_{n+1} - f_n, \dots,$$

are called the *forward finite differences of the first order*; the quantities

$$\Delta^2 f_0 = \Delta f_1 - \Delta f_0, \quad \Delta^2 f_1 = \Delta f_2 - \Delta f_1, \dots, \Delta^2 f_n = \Delta f_{n+1} - \Delta f_n, \dots,$$

are called the *forward finite differences of the second order*, and so on. Also,

$$\Delta^2 f_0 = \Delta(\Delta f_0) = \Delta f_2 - \Delta f_1 = f_3 - 2f_2 + f_1,$$

$$\Delta^2 f_i = f_{i+2} - 2f_{i+1} + f_{i-1},$$

$$\Delta^3 f_1 = \Delta(\Delta^2 f_1) = f_4 - 3f_3 + 3f_2 - f_1,$$

$$\Delta^3 f_i = f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i,$$

and, in general,

$$\Delta^n f_i = f_{i+n} - \binom{n}{1} f_{i+n-1} + \binom{n}{2} f_{i+n-2} - \cdots + (-1)^{n-1} \binom{n}{n-1} f_{i+1} + (-1)^n f_i. \quad (1.3.1)$$

This provides the recursive relation

$$\Delta^n f = f_n - \binom{n}{1} f_{n-1} + \binom{n}{2} f_{n-2} - \binom{n}{3} f_{n-3} + \cdots + (-1)^n f_0. \quad (1.3.2)$$

If we introduce the operator \mathcal{H} which increases the argument by h , i.e., $\mathcal{H}f(x) = f(x+h)$, or $\mathcal{H}f_k = f_{k+1}$, then the relation (1.3.2) can be written symbolically as

$$\Delta^n f_0 = (\mathcal{H} - 1)^n f_0. \quad (1.3.3)$$

Note that any value of the function f_n can also be expressed in terms of f_0 and the forward finite differences $\Delta f_0, \Delta^2 f_0, \dots$, by using the relation

$$f_n = f_0 + \binom{n}{1} \Delta f_0 + \binom{n}{2} \Delta^2 f_0 + \cdots + \Delta^n f_0, \quad (1.3.4)$$

or symbolically by

$$f_n = (1 + \Delta)^n f_0. \quad (1.3.5)$$

Also, note that

$$\begin{aligned} \Delta(ax^n) &= a(x+h)^n - ax^n = (anh)x^{n-1} + \text{terms of lower degree in } x, \\ \Delta(anhx^{n-1}) &= an(n-1)h^2x^{n-2} + \text{terms of lower degree in } x, \\ &\dots \\ \Delta p_n(x) &= \Delta(a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n) \\ &= a_0nhx^{n-1} + \text{terms of lower degree in } x, \end{aligned}$$

and thus,

$$\Delta^n p_n(x) = a_n n!. \quad (1.3.6)$$

The *backward difference operator* ∇ is defined by

$$\begin{aligned} \nabla f_i &= f_i - f_{i-1}, \\ \nabla^{n+1} f_i &= \nabla(\nabla^n f_i). \end{aligned}$$

Note that the forward and backward difference formulas represent the same polynomial. Also, $\nabla f_n, \nabla^2 f_n, \nabla^3 f_n, \dots$ denote the same numbers as $\Delta f_{n-1}, \Delta f_{n-2}, \Delta f_{n-3}, \dots$.

The *central differences* are defined by

$$\begin{aligned}
 \delta f_{n+1/2} &= \delta_{n+1/2} = \delta_{n+1/2}^1 = f_{n+1} - f_n, \\
 \delta_n^2 &= \delta_{n+1/2}^1 - \delta_{n-1/2}^1 = f_{n+1} - 2f_n + f_{n-1}, \\
 \delta_{n+1/2}^3 &= \delta_{n+1}^2 - \delta_n^2 = f_{n+2} - 3f_{n+1} + 3f_n - f_{n-1}, \\
 &\dots \quad \dots \quad \dots \quad \dots \quad \dots \quad \dots \quad \dots, \\
 \delta_n^{2k} &= \sum_{j=0}^{2k} (-1)^j \binom{2k}{j} f_{n+k-j}, \\
 \delta_{n+1/2}^{2k+1} &= \sum_{j=0}^{2k+1} (-1)^j \binom{2k+1}{j} f_{n+k+1-j}, \\
 \delta_{1/2n}^k &= \Delta_{1/2(n-k)}^k \quad \text{if } n \text{ and } k \text{ have the same parity.}
 \end{aligned}$$

1.3.2. Divided Differences. In the case when the values of the argument are unequally spaced, the finite differences are replaced by quantities which are called *divided differences*. Let $x_0, x_1, x_2, \dots, x_n, \dots$ denote the arbitrary values of the argument. The divided differences of the first order are defined by

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}, \quad f[x_1, x_2] = \frac{f(x_2) - f(x_1)}{x_2 - x_1}, \quad \dots;$$

the divided differences of the second order by

$$\begin{aligned}
 f[x_0, x_1, x_2] &= \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}, \\
 f[x_1, x_2, x_3] &= \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}, \quad \dots;
 \end{aligned}$$

the divided differences of the third order by

$$f[x_0, x_1, x_2, x_3] = \frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0}, \quad \dots;$$

and so on. This leads to the formula

$$f[x_0, x_1, \dots, x_n] = \frac{f[x_0, \dots, x_n] - f[x_0, \dots, x_{n-1}]}{x_n - x_0}. \quad (1.3.7)$$

Note that, in general, the divided difference $f[x_0, x_1, \dots, x_n]$ is a linear function of $f(x_0), \dots, f(x_n)$, and

$$f[x_0, x_1, \dots, x_n] = \sum_{k=0}^n \frac{f(x_k)}{(x_k - x_0) \dots (x_k - x_{k-1})(x_k - x_{k+1}) \dots (x_k - x_n)}. \quad (1.3.8)$$

If we use the backward difference operator, we obtain the backward difference form

$$p_n(x) = p_n(x_n + sh) = \sum_{j=0}^n (-1)^j \binom{-s}{j} \nabla^j f_n. \quad (1.3.15)$$

The error term in (1.3.13) is given by

$$f(x) - p_n(x) = (-1)^{n+1} h^{n+1} \binom{s}{n+1} f^{(n+1)}(\xi_s). \quad (1.3.16)$$

Sometimes it is useful in applications to relate finite and divided differences to derivatives. Thus, assuming that the points x_0, x_1, \dots, x_n lie on the interval $[a, b]$, we have

$$\begin{aligned} f(x_0, x_1, \dots, x_n) &= \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} f^{(n)} \left(x_0 + \sum_{k=1}^n t_k (x_k - x_{k-1}) \right) \times \\ &\quad \times dt_n \cdots dt_2 dt_1. \end{aligned} \quad (1.3.17)$$

This result can be proved by induction (see Krylov 1962). Notice that the region of integration in formula (1.3.17) is a simplex in the n -dimensional space (t_1, t_2, \dots, t_n) , such that

$$0 \leq t_n \leq t_{n-1} \leq \cdots \leq t_1 \leq 1. \quad (1.3.18)$$

The volume of this simplex is

$$\int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} dt_n \cdots dt_2 dt_1 = \frac{1}{n!}.$$

Moreover, the quantity

$$\begin{aligned} \nu &\equiv x_0 + \sum_{k=1}^n t_k (x_k - x_{k-1}) \\ &= (1 - t_0) x_0 + (t_1 - t_2) x_1 + \cdots + (t_{n-1} - t_n) x_{n-1} + t_n x_n, \end{aligned}$$

which is the argument in the integrand in formula (1.3.17), clearly shows that the multipliers of all x_k are nonnegative, and since the sum of these multipliers is unity, the quantity ν is a weighted average of the points x_k , $k = 0, 1, \dots, n$. Thus, the quantity ν lies in the interval $[a, b]$, and, therefore, a point in the interior of the simplex (1.3.18) corresponds to an interior point of the interval $[a, b]$. Hence, after applying the mean-value theorem to the integral in formula (1.3.17), we find that if $f(x)$ has a continuous derivative of order n on $[a, b]$, then there exists an interior point ν of $[a, b]$ such that

$$f(x_0, x_1, \dots, x_n) = \frac{f^{(n)}(\nu)}{n!}. \quad (1.3.19)$$

Thus, Eqs (1.3.12), (1.3.17), and (1.3.19) provide the relationship between the finite differences and derivatives, which is

$$\Delta^n f_0 = n! h^n \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} f^{(n)}\left(x_0 + h \sum_{k=1}^n t_k\right) \times \quad (1.3.20)$$

$$\times dt_n \cdots dt_2 dt_1 = h^n f^{(n)}(\nu), \quad x_0 < \nu < x_0 + n h.$$

1.4. Interpolation

In [Chapter 2](#) we will discuss certain quadrature rules which are obtained by integrating interpolating polynomials. These rules are called *interpolatory quadrature rules*. Therefore, we first introduce the concept of interpolation and some related results.

The problem of interpolation stated in a simple form is as follows. When a function has been obtained as a set of tabulated values, we may seek this function at a value of the argument which is different from the tabulated data. This problem also includes *extrapolation*. Let $\{f_0(x), f_1(x), \dots, f_n(x)\}$ denote a set of prescribed basic coordinate functions, tabulated at the points x_0, x_1, \dots, x_n in the interval $[a, b]$ for $a \leq x \leq b$. Then we seek an approximation $f(x)$ of the form

$$f(x) \approx (Af)(x) = \sum_{i=1}^n a_i f_i(x), \quad (1.4.1)$$

where the values $a_i, i = 0, 1, \dots, n$, may be computed from the tabulated values of $f(x)$ in some prescribed manner. The function $(Af)(x)$ in Eq (1.4.1) is known as an *interpolant* and is often denoted by $P_{0,1,\dots,n}(x)$. Suppose that the function $f(x)$ is tabulated at some distinct points x_0, x_1, \dots, x_n in the interval $[a, b]$. Assume that $\det[f_i(x_j)] \neq 0$. Then there exist unique values a_0, a_1, \dots, a_n in Eq (1.4.1) such that

$$f_j \equiv f(x_j) = \sum_{i=0}^n a_i f_i(x_j) \quad \text{for } j = 0, 1, \dots, n.$$

If we take $f_r(x)$ as a polynomial of degree r in x , then the interpolant is a polynomial of degree at most n .

1.4.1. Lagrangian Polynomial. The Lagrangian polynomial, which is widely used in these problems, has the interpolant defined by

$$(Af)(x) \equiv P_{0,1,\dots,n}(x) = \sum_{j=0}^n l_j(x) f(x_j), \quad (1.4.2)$$

where

$$l_j(x) = \prod_{\substack{i=0 \\ i \neq j}}^n \frac{x - x_i}{x_j - x_i}. \quad (1.4.3)$$

The formula (1.4.2) can be written explicitly as

$$\begin{aligned} P_{0,1,\dots,n}(x) &= \frac{(x - x_1)(x - x_2) \dots (x - x_n)}{(x_0 - x_1)(x_0 - x_2) \dots (x_0 - x_n)} f_0 \\ &+ \frac{(x - x_0)(x - x_2) \dots (x - x_n)}{(x_1 - x_0)(x_1 - x_2) \dots (x_1 - x_n)} f_1 \\ &+ \dots + \frac{(x - x_0)(x - x_1) \dots (x - x_{n-1})}{(x_n - x_0)(x_n - x_1) \dots (x_n - x_{n-1})} f_n, \end{aligned} \quad (1.4.4)$$

where $f_j = f(x_j)$, $j = 0, 1, \dots, n$, and the error $E(x) = f(x) - (Af)(x)$ in this interpolation formula is given by

$$E(x) = (x - x_0)(x - x_1) \dots (x - x_n) \frac{f^{n+1}(\xi)}{(n+1)!}, \quad a < \xi < b, \quad (1.4.5)$$

if $f^{n+1}(\xi)$ is continuous and ξ depends on x . For interpolation with the Lagrangian polynomials, see [interp0.f90](#), [interp.m](#) and [interp.nb](#) on the CD-R.

EXAMPLE 1.4.1. (a) **Constant interpolation:** $n = 0$, $x_0 = a$, $P_0(x) = f(a)$, $a \leq x \leq b$, and $E(x) = (x - a)f'(\xi)$, $a < \xi < b$, if $f'(\xi)$ is continuous and ξ depends on x .

(b) **Constant interpolation:** $n = 0$, $x_0 = \frac{a+b}{2}$, $P_0(x) = f\left(\frac{a+b}{2}\right)$, $a \leq x \leq b$, and $E(x) = \left(x - \frac{a+b}{2}\right)f'(\nu)$, $a < \nu < b$, if $f'(\nu)$ is continuous and ν depends on x .

(c) **Linear interpolation:** $n = 1$, $x_0 = a$, $x_1 = b$,

$$P_{0,1}(x) = \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b), \quad a \leq x \leq b,$$

and $E(x) = \frac{1}{2}(x-a)(x-b)f''(\eta)$, $a < \eta < b$, if $f''(\eta)$ is continuous and η depends on x .

(d) **Quadratic interpolation:** $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2} \equiv c$, $x_2 = b$,

$$\begin{aligned} P_{0,1,2}(x) &= \frac{(x-c)(x-b)}{(a-c)(a-b)} f(a) + \frac{(x-a)(x-b)}{(c-a)(c-b)} f(c) \\ &+ \frac{(x-a)(x-c)}{(b-a)(b-c)} f(b), \quad a \leq x \leq b, \end{aligned}$$

and $E(x) = \frac{1}{6} (x - a)(x - c)(x - b)f'''(\xi)$, $a < \xi < b$, if $f'''(\xi)$ is continuous and ξ depends on x . ■

1.4.2. Neville’s Method. (Also known as Neville-Aitken method, see [Phillips and Taylor 1996](#).) The Lagrangian polynomial method often fails to tell us which degree of polynomials to use. If the degree is too low, the interpolating polynomial does not give a good estimate for $f(x)$, and if the degree is too high, the polynomial value may undergo oscillations. This means that we cannot predict how many points x_k will be needed to achieve the desired precision in interpolation. Suppose we find that the required precision is not achieved for the number of points x_k first chosen. Then we must use one or more additional points. But introducing one or more points completely changes all the terms in (1.4.4).

Neville’s method computes the interpolated value with polynomials of successively higher degree and stops when the successive values converge to a common value. It uses the above Lagrangian formula for the linear interpolation, i.e.,

$$f(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 = \frac{(x - x_1) f_0 + (x_0 - x) f_1}{x_0 - x_1}. \tag{1.4.6}$$

NEVILLE’S TABLE. Since each successive value is obtained by linear interpolation, we will denote the interpolant $P_{0,1,2,\dots,i}$ associated with f_i in short by P_{i0} . Then, after rearranging the tabulated value in order of closeness to the value of x where $f(x)$ is to be interpolated, we construct a table for the linear interpolants for $i = 0, 1; i = 1, 2; i = 2, 3$; and so on. The successive computed values are arranged in columns, such that the next column contains linear interpolation values from the previous column for $i = 0, 2, \dots$, and the next column uses these values. This process is continued until it runs out of the interpolation pairs. The formula for computing the values in the Neville’s table is

$$P_{ij} = \frac{(x - x_i) P_{i+1,j-1} + (x_{i+j} - x) P_{i,j-1}}{x_{i+j} - x_i}. \tag{1.4.7}$$

To implement this method, see [neville.f90](#), [neville.m](#) and [neville.nb](#) on the CD-R.

EXAMPLE 1.4.2. Consider the tabulated data:

Table 1.4.1.

x	10.2	23.5	33.4	42.7	54.1
$f(x)$	0.98419	0.91706	0.83485	0.73491	0.58637

and interpolate $f(29)$.

First, we arrange the values in order of closeness to $x = 29$; this is done by using the values of $|x - x_i|$.

Table 1.4.2.

i	$ x - x_i $	x_i	P_{i0}
0	4.4	33.4	0.83485
1	5.5	23.5	0.91706
2	13.7	42.7	0.73491
3	18.8	10.2	0.98419
4	25.1	54.1	0.58637

By using formula (1.4.7) with $x = 29$, the Neville's table is

Table 1.4.3.

i	x_i	P_{i0}	P_{i1}	P_{i2}	P_{i3}	P_{i4}
0	33.4	0.83485	0.87138	0.87446	0.87466	0.87462
1	23.5	0.91706	0.86488	0.87517	0.87450	
2	42.7	0.73491	0.83999	0.87143		
3	10.2	0.98419	0.81382			
4	54.1	0.58637				

The top row of the above table represents the Lagrangian interpolants at $x = 29$, where the second subscript of P_{ij} is equal to the degree of the polynomial. The values converge to 0.87462, which is obtained for $j = 4$. The original data contains the values of $f(x) = \cos x$, where x is in degrees; the exact value of $\cos 29^\circ = 0.87462$. Note that the rearrangement of the table in the order of closeness to $x = 29$ brings out the convergence faster by centering the x -value relative to the prescribed data. ■

1.4.3. Osculating Polynomials. The expression for $l_j(x)$ in (1.4.3) or the interpolant (1.4.4) becomes indeterminate if some of the points x_i coincide. In such cases we must find a new form for $P_{0,1,\dots,n}(x)$. The interpolant is then called an *osculating polynomial*. Some examples of osculating polynomials are given below.

EXAMPLE 1.4.3. (a) Truncated Taylor Series, when $x_0 = x_1 = \dots = x_n = a$. The interpolant is

$$P_{0,\dots,0}(x) = f(a) + (x-a)f'(a) + \dots + \frac{(x-a)^n}{n!} f^{(n)}(a),$$

and the error is given by

$$\begin{aligned} E(x) &= f(x) - P_{0,\dots,0}(x) = \frac{1}{n!} \int_a^x (x-t)^n f^{(n+1)}(t) dt \\ &= \frac{(x-a)^{n+1}}{(n+1)!} f^{(n+1)}(\xi), \quad a < \xi < x, \end{aligned}$$

if $f^{(n+1)}(x)$ is continuous for $a \leq x \leq b$, and ξ depends on x .

(b) **Two-Point Taylor Interpolation.** Let $n = 2m - 1$, $x_0 = x_1 = \dots = x_{m-1} = a$, and $x_m = x_{m+1} = \dots = x_{2m-1} = b$. Then the error is given by

$$E(x) = f(x) - P_{0,\dots,0,n,\dots,n}(x) = \frac{(x-a)^m(x-b)^m}{(2m)!} f^{(2m)}(\eta), \quad a < \eta < b,$$

if $f^{(2m)}(x)$ is continuous, and η depends on x (see [Davis 1976](#), p.37). ■

Instead of approximating $f(x)$ by an osculating polynomial over the interval $[a, b]$, we partition the interval, say, by $a = x_0 < x_1 < \dots < x_N = b$, and interpolate $f(x)$ separately over each subinterval $[x_i, x_{i+1}]$ by a suitable interpolating polynomial. This method is known as the *piecewise-polynomial interpolation*. The method simplifies if $x_i = x + ih$, where $h = (b-a)/N$. The resulting interpolant is denoted by $P_{0,1,\dots,N}(x)$ for each piecewise interpolating polynomial.

EXAMPLE 1.4.4. (see [Baker 1978](#), p.90) In the examples (a)–(c) of piecewise-polynomial interpolations given below, it is assumed that $x_i = x_0 + i h$.

(a) **Piecewise-Constant Interpolation** (see [Example 1.4.1](#)).

$$f(x) \approx (Af)(x) = \begin{cases} f(x_i) & \text{if } x_i \leq x < x_{i+1}, i \neq N-1, \\ f(x_{N-1}) & \text{if } x_{N-1} \leq x \leq x_N; \end{cases}$$

$$\text{error} = |f(x) - (Af)(x)| \leq h \max_{a \leq \xi \leq b} |f'(\xi)| \quad \text{if } f'(\xi) \text{ is continuous.}$$

(b) **Piecewise-Linear Interpolation** (see [Example 1.4.1](#)).

$$f(x) \approx (Af)(x) = \frac{x - x_i}{h} f(x_{i+1}) - \frac{x - x_{i+1}}{h} f(x_i), \quad x_i \leq x \leq x_{i+1},$$

$$\text{error} = |f(x) - (Af)(x)| \leq \frac{h^2}{2} \max_{a \leq \xi \leq b} |f''(\xi)| \quad \text{if } f''(\xi) \text{ is continuous.}$$

(c) Take $(Af)(x)$ as a piecewise two-point Taylor interpolating polynomial (see [Example 1.4.3](#)) of degree $n = 2m - 1$. Then the approximation $A(f)(x)$ has a continuous $(m+1)$ -th derivative. If $m = 2$, then $n = 3$, and we obtain a polynomial which is piecewise cubic and has a continuous first derivative with error

$$\text{error} = |f(x) - (Af)(x)| = \frac{(x-a)^2(x-b)^2}{4!} f^{(iv)}(\xi), \quad a < \xi < b. \quad \blacksquare$$

1.4.4. Richardson Extrapolation. This method is used for the numerical differentiation of a known function $f(x)$. It uses smaller h -values rather than the larger ones as is the case when the function is known only in a tabulated form. Thus, we start with an arbitrary value of h and compute

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}.$$

Then we take the value of h half as large and compute the second value of $f'(x)$, and a third value with half of the previous h -value, and so on, for the first approximations; we stop only when the computed values do not differ from each other. For the subsequent approximations we extrapolate by using the formula

$$\text{better estimate} = \text{second value} + \frac{1}{2^n - 1} (\text{second value} - \text{first value}), \quad (1.4.8)$$

where the ‘second value’ refers to the value of $f'(x)$ computed with the halved h -value. Since the first approximations have errors of order $O(h^4)$, so $n = 4$ in formula (1.4.8). The higher-order extrapolations use the h -values halved at each stage. The convergence is achieved when two consecutive approximations yield the same result. For clarity the results of each extrapolation are presented as a table. To create a Richardson extrapolation table, see [extrapol.f90](#), [extrapol.m](#) and [extrapol.nb](#) on the CD-R.

EXAMPLE 1.4.5. Use Richardson extrapolation for $f(x) = x^2 \sin x$ to compute $f'(1.5)$, taking $h = 0.1$ (see Table 1.4.5). The exact value is $f'(1.5) = 3.15164$. For computational details, see [richard.nb](#) on the CD-R. ■

Table 1.4.5.

3.13713						
3.14801	3.14874					
3.15074	3.15092	3.15106				
3.15142	3.15146	3.15150	3.15153			
3.15159	3.15160	3.15161	3.15161	3.15162		
3.15163	3.15163	3.15163	3.15164	3.15164	3.15164	
3.15164	3.15164	3.15164	3.15164	3.15164	3.15164	3.15164

1.4.5. Error Bounds in Polynomial Interpolation. Let $f(x) \in C^{n+1}[a, b]$, and let its interpolant $P_{0,1,\dots,n}(x)$ be a polynomial of degree at most n such that both the function $f(x)$ and the interpolant have the same values at the points $x_0, x_1, \dots, x_n \in [a, b]$. Then, in view of the Rolle’s theorem we have for $a \leq x \leq b$

$$f(x) - P_{0,1,\dots,n}(x) = \prod_{i=0}^n (x - x_i) \frac{f^{(n+1)}(\xi)}{(n+1)!}, \quad a < \xi < b, \quad (1.4.9)$$

where ξ depends on x , and each point x_i is counted according to its multiplicity. Then we obtain an error bound

$$\|f(x) - P_{0,1,\dots,n}(x)\|_\infty \leq \left\| \prod_{i=0}^n (x - x_i) \right\|_\infty \frac{\|f^{(n+1)}(x)\|_\infty}{(n+1)!}, \quad (1.4.10)$$

provided $\|f^{(n+1)}(x)\|_\infty$ is known. However, in those cases when $f^{(n+1)}(x)$ does not exist or cannot be easily estimated, an error bound can be found with a lower order estimate.

In the case of distinct points $x_i, i = 0, 1, \dots, n$, the following result is useful. Let $f(x) \in C[a, b]$, and denote

$$E_n(f) = \inf_{p_n} \left\{ \sup_{a \leq x \leq b} |f(x) - p_n(x)| \right\} = \inf_{p_n} \|f(x) - p_n(x)\|_\infty, \quad (1.4.11)$$

where $p_n(x)$ is a polynomial of degree n . The modulus of continuity $\omega(f; \delta)$ associated with the function $f(x)$ is defined by

$$\omega(f; \delta) = \sup \{ |f(x) - f(y)| \text{ such that } a \leq x, y \leq b, |x - y| < \delta \}. \quad (1.4.12)$$

Then, we have

$$E_n(f) \leq \frac{\pi(b-a)L}{4(n+1)}, \quad (1.4.13)$$

if

$$f(x_1) - f(x_2) \leq L|x_1 - x_2| \quad (1.4.14)$$

holds for all $x_1, x_2 \in [a, b]$; and

$$E_n(f) \leq \left[\frac{\pi(b-a)}{4} \right]^k \frac{\|f^{(k)}(x)\|_\infty}{(n+1)n \dots (n-k+2)}, \quad (1.4.15)$$

if $f^{(k)}(x)$ is bounded on $[a, b]$ and $n \geq k$. The bound (1.4.13) is known as *Jackson's theorem* (see [Cheney](#) 1966, [Rivlin](#) 1981). It says that $f(x)$ is Lipschitz-continuous when it satisfies the Lipschitz condition (1.4.14). Also, the results (1.4.13) imply that

$$E_n(f) \leq \omega\left(f; \frac{\pi(b-a)}{2(n+1)}\right). \quad (1.4.16)$$

The bound (1.4.15) is proved in Cheney (1966, p. 148).

If we use a polynomial $r_n(x)$ of degree n for which $E_n(f) = \|f(x) - r_n(x)\|_\infty$, then, in view of (1.4.2), for distinct points x_0, x_1, \dots, x_n , we obtain

$$\begin{aligned} \|f(x) - P_{0,1,\dots,n}(x)\|_\infty &= \|f(x) - \sum_{j=0}^n l_j(x) f(x_j)\|_\infty \\ &\leq \|f(x) - r_n(x)\|_\infty + \left\| \sum_{j=0}^n l_j(x) \{r_n(x_j) - f(x_j)\} \right\|_\infty \\ &\leq \left\{ 1 + \left\| \sum_{j=0}^n |l_j(x)| \right\|_\infty \right\} E_n(f). \end{aligned} \quad (1.4.17)$$

The number

$$L_n = \left\| \sum_{j=0}^n |l_j(x)| \right\|_\infty \quad (1.4.18)$$

is called the *Lebesgue constant for polynomial interpolation*. The size of this number depends on n and the distribution of the points $x_j, j = 0, 1, \dots, n$, and the points a and b , since $\|f(x)\|_\infty = \sup_{a \leq x \leq b} |f(x)|$.

SPECIAL CASES.

(i) For $a = -1, b = 1$, and $x_j = \frac{\cos(2j+1)\pi}{2(n+1)}, j = 0, 1, \dots, n$, the number $L_n \leq 2\pi \ln n + 4$ (see [Powell 1968](#), [Rivlin 1981](#)). Note that $\frac{1}{n} \ln n \rightarrow 0$ as $n \rightarrow \infty$. Then with the above choice of x_j and $[a, b] = [-1, 1]$, we have

$$\lim_{n \rightarrow \infty} \|f(x) - P_{0,1,\dots,n}(x)\|_\infty = 0$$

provided that $f(x)$ is Lipschitz-continuous. The points x_j are the zeros of the Chebyshev polynomial of the first kind $T_{n+1}(x)$, which is defined by $T_{n+1}(x) = \cos[(n+1) \arccos x]$ if $|x| \leq 1$ (see (1.4.2)).

If we take $a = 0, b = 1$, we obtain the same result as in case (i) provided x_j are taken as the zeros of the shifted Chebyshev polynomial $T_{n+1}^*(x) = T_{n+1}(2x - 1)$, since the value of L_n is the same in both cases.

(ii) For the general distribution of the points $x_j, j = 0, 1, \dots, n$, and an arbitrary function $f(x) \in C[a, b]$, it is not true that $\lim_{n \rightarrow \infty} \|f(x) - P_{0,1,\dots,n}(x)\|_\infty = 0$ (see [Natanson 1964](#), and [Cheney 1966](#)), but $P_{0,1,\dots,n}(x)$ does converge in the mean to $f(x)$ (see [Natanson 1964](#), p. 56). Note that if $a = -1, b = 1$, and x_j are the zeros of the Legendre polynomial $P_{n+1}(x)$, then

$$\lim_{n \rightarrow \infty} \|f(x) - P_{0,1,\dots,n}(x)\|_\infty = 0.$$

1.4.6. Newton-Gregory Forward Polynomial. This polynomial passes through a finite set of equidistant points, and is defined by

$$p_n(x_s) = f_0 + \binom{s}{1} \Delta f_0 + \binom{s}{2} \Delta^2 f_0 + \dots + \binom{s}{n-1} \Delta^{n-1} f_0 + \Delta^n f_0, \quad (1.4.19)$$

where h is prescribed, $s = (x - x_0)/h$, and

$$\binom{s}{j} = \frac{s!}{(s-j)!j!} = \frac{s(s-1)\dots(s-j+1)}{j!}.$$

The error in (1.5.9) is given by

$$E(x_s) = h^{n+1} \binom{s}{n+1} f^{n+1}(\xi), \quad a < \xi < b. \quad (1.4.20)$$

1.5. Semi-Infinite Interval

Let the interval $[0, \infty)$ be partitioned into equal subintervals of length $h > 0$ by the points $x_k = kh$, $k = 0, 1, 2, \dots$, and let the values of a function f at these points be denoted by $f(x_k) = f(kh) = f_k$.

1.5.1. Linear Interpolation. Consider the interval $[kh, (k+1)h]$, and linearly interpolate a function $f(x)$ with respect to the values at the two endpoints:

$$f(x) = \frac{x - (k+1)h}{-h} f_k + \frac{x - kh}{h} f_{k+1} + E_k(x, f). \quad (1.5.1)$$

Then, if $f \in C^2[kh, (k+1)h]$, the error $E_k(x, f)$ is given by (Krylov and Skoblya 1977, p. 171)

$$E_k(x, f) = h^2 \int_0^1 f''(kh + \tau h) [(\xi - \tau)U(\xi - \tau) - \xi(1 - \tau)] d\tau, \quad (1.5.2)$$

where $x = x_k + \xi h = (k + \xi)h$, $0 \leq \xi < 1$.

1.5.2. Quadratic Interpolation. Consider the interval $[kh, (k+2)h]$ of length $2h$, and interpolate the function f with respect to the values f_k , f_{k+1} , and f_{k+2} at the points kh , $(k+1)h$, and $(k+2)h$ with a polynomial $p_2(x)$ of degree 2. Then the parabolic interpolation is

$$\begin{aligned} f(x) = & \frac{(x - x_{k+1})(x - x_{k+2})}{(-h)(-2h)} f_k + \frac{(x - x_k)(x - x_{k+2})}{(-h)(h)} f_{k+1} \\ & + \frac{(x - x_k)(x - x_{k+1})}{(h)(2h)} f_{k+2} + E_k(x, f), \end{aligned} \quad (1.5.3)$$

which is analogous to the Newton-Cotes parabolic rule (see §2.4.) To find the error $E_k(x)$, we use the Taylor's formula with remainder in the form of an integral:

$$\begin{aligned} f(x) = & f_k + (x - x_k) f'_k + \frac{1}{2} (x - x_k)^2 f''_k + \frac{1}{2} \int_{x_k}^x f'''(t)(x - t)^2 dt \\ = & p_2(x) + \frac{1}{2} \int_{x_k}^{x_{k+2}} f'''(t)(x - t)^2 U(x - t) dt = p_2(x) + q(x). \end{aligned} \quad (1.5.4)$$

Since the polynomial $p_2(x)$ is interpolated exactly, the interpolation errors of $f(x)$ and $q(x)$ are the same. Thus,

$$\begin{aligned} E_k(x, f) = & \frac{1}{2} \int_{x_k}^{x_{k+2}} f'''(t) [(x - t)^2 U(x - t) \\ & + \frac{(x - x_k)(x - x_{k+2})}{h^2} (x_{k+1} - t)^2 U(x_{k+1} - t) \\ & - \frac{1}{2} \frac{(x - x_k)(x - x_{k+1})}{h^2} (x_{k+2} - t)^2] dt. \end{aligned} \quad (1.5.5)$$

Since $U(x_k - t) = 0$, and $U(x_{k+2} - t) = 1$ for all $t < x_{k+2}$, we obtain the simplified expression for $E_k(x)$ by introducing new variables ξ and τ by setting $x = x_k + \xi h$ and $t = x_k + \tau h$, $0 \leq \xi, \tau < 2$. Thus,

$$E_k(x, f) = \frac{h^3}{2} \int_0^2 f'''(x_k + \tau h) [(\xi - \tau)^2 U(\xi - \tau) + \xi(\xi - 2)(1 - \tau)^2 U(1 - \tau) - \frac{1}{2} \xi(\xi - 1)(2 - \tau)^2] dt. \quad (1.5.6)$$

1.5.3. Cubic Interpolation. There are three cases, as follows.

1.5.3(a) Cubic Interpolation with Four Single Points. The rule for the interpolation of degree 3 are analogous to the Newton-Cotes 3/8-rule (see §2.4). We take 4 points x_k, x_{k+1}, x_{k+2} , and x_{k+3} , and interpolate f with respect to values at these points:

$$\begin{aligned} f(x) = & \frac{(x - x_{k+1})(x - x_{k+2})(x - x_{k+3})}{(-h)(-2h)(-3h)} f_k \\ & + \frac{(x - x_k)(x - x_{k+2})(x - x_{k+3})}{h(-h)(h)} f_{k+1} \\ & + \frac{(x - x_k)(x - x_{k+1})(x - x_{k+3})}{(-h)(h)(2h)} f_{k+2} \\ & + \frac{(x - x_k)(x - x_{k+1})(x - x_{k+2})}{(3h)(2h)(h)} f_{k+3} + E_k(x, f), \end{aligned} \quad (1.5.7)$$

1.5.3(b) Cubic Interpolation with Two Double Points. Over the interval $[kh, (k+1)h]$ interpolate f at the points x_k , and x_{k+1} with respect to the values f_k, f_{k+1}, f'_k , and f'_{k+1} at these points by using a polynomial of degree 3:

$$\begin{aligned} f(x) = & \frac{(x - x_{k+1})^2}{h^2} \left[\left(1 + 2 \frac{x - x_k}{h} \right) f_k + (x - x_k) f'_k \right] \\ & + \frac{(x - x_k)^2}{h^2} \left[\left(1 - 2 \frac{x - x_{k+1}}{h} \right) f_{k+1} + (x - x_{k+1}) f'_{k+1} \right] + E_k(x, f). \end{aligned} \quad (1.5.8)$$

By using the Taylor's formula we get

$$\begin{aligned} f(x) = & f_k + (x - x_k) f'_k + \frac{1}{2} (x - x_k)^2 f''_k \\ & + \frac{1}{6} (x - x_k)^3 f'''_k + \frac{1}{6} \int_{x_k}^x f^{(4)}(t)(x - t)^3 dt \\ = & p_3(x) + \frac{1}{6} \int_{x_k}^{x_{k+1}} f^{(4)}(t)(x - t)^3 U(x - t) dt, \end{aligned} \quad (1.5.9)$$

where the error $E_k(x, f)$ is given by

$$\begin{aligned}
 E_k(x, f) &= \frac{1}{6} \int_{x_k}^{x_{k+1}} f^{(4)}(t) \left\{ (x-t)^3 U(x-t) \right. \\
 &\quad \left. - \frac{(x-x_k)^2}{h^2} \left[\left(1 - 2\frac{x-x_{k+1}}{h}\right) (x_{k+1}-t)^3 \right. \right. \\
 &\quad \left. \left. + 3(x-x_{k+1})(x_{k+1}-t)^2 \right] \right\} dt \\
 &= \frac{h^4}{6} \int_0^1 f^{(4)}(x_k + \tau h) \left\{ (\xi - \tau)^3 U(\xi - \tau) \right. \\
 &\quad \left. - \xi^2 [(3 - 2\xi)(1 - \tau)^3 + 3(\xi - 1)(1 - \tau)^2] \right\} d\tau \\
 &= \frac{h^4}{6} \int_0^1 f^{(4)}(x_k + \tau h) \left\{ (\xi - \tau)^3 U(\xi - \tau) \right. \\
 &\quad \left. + \xi^2 (1 - \tau)^2 [(3 - 2\xi)\tau - \xi] \right\} d\tau, \tag{1.5.10}
 \end{aligned}$$

where we have set $x = x_k + \xi h$, $t = x_k + \tau h$, $0 \leq \xi, \tau \leq 1$.

1.5.3(c) Cubic Interpolation with Three Double Points. Over the interval $[kh, (k+1)h]$ interpolate f at the points x_k, x_{k+1} , and x_{k+2} with respect to the values $f_k, f_{k+1}, f'_k, f'_{k+1}, f_{k+2}$, and f'_{k+2} at these points:

$$\begin{aligned}
 f(x) &= \sum_{j=0}^2 \frac{\pi_k^2(x)}{(x-x_{k+j})^2 [\pi_k(x_{k+j})]^2} \left\{ \left[1 - \frac{\pi_k''(x_{k+j})}{\pi_k'(x_{k+j})} (x-x_{k+j}) \right] f_{k+j} \right. \\
 &\quad \left. + (x-x_{k+j}) f'_{k+j} \right\} + E_k(x, f), \tag{1.5.11}
 \end{aligned}$$

where $\pi(x) = (x-x_k)(x-x_{k+1})(x-x_{k+2})$. The interpolation error is given by

$$E_k(x, f) = \frac{\pi^2(x)}{6!} f^{(4)}(x_k + \theta_k h), \quad 0 \leq \theta_k < 2. \tag{1.5.12}$$

1.5.4. Transformation to the interval $[0, 1]$. Consider the functions f that satisfy the condition $|f(x)| \leq A x^{-s}$, $s > 1$, $A > 0$, for large values of x . Among such functions we choose those functions F that can be represented in the form

$$F(x) = (1+x)^s f(x), \quad s > 1,$$

where $f \in C[0, \infty)$, such that $\lim_{x \rightarrow \infty} F(x) = F(\infty) < +\infty$. Thus, such functions F are regarded as continuous on the closed interval $[0, \infty]$ and the finite limit value $F(\infty)$ is taken as its value at the point at infinity. For the sake of simplicity, we consider as

the basic function the system of simple fractions $1/(1+x)^m$, $m = 0, 1, 2, \dots$, and interpolate by using the polynomials in the argument $1/(1+x)$, i.e.,

$$p_n(x) = \sum_{m=0}^n \frac{a_m}{(1+x)^m}. \quad (1.5.13.)$$

These polynomials form a complete system in the metric in the set of functions $F(x) \in C[0, \infty]$. Then the transformation $z = \frac{1}{1+x}$ carries the half-axis $[0, \infty]$ into the interval $[0, 1]$, and the function $F(x)$ which is continuous on $[0, \infty]$ goes into a function $G(x)$ continuous on $[0, 1]$ on the real z -axis, and the rational functions $p_n(x)$ go into the polynomials $p_n(z)$, which, by Weierstrass' theorem, form a complete set of algebraic polynomials in the class of functions continuous on a finite closed interval.

If on the half-axis $[0, \infty)$ we take $n+1$ points x_k such that $0 \leq x_0 < x_1 < \dots < x_n < \infty$ and choose the coefficients a_k of the function $p_n(x)$ so that its values at the points x_k coincide with the values of F :

$$p_n(x_k) = \sum_{i=0}^n a_i (1+x_k)^{-i} = F(x_k), \quad k = 0, 1, \dots, n. \quad (1.5.14)$$

Then we obtain a linear system of equations to determine the coefficients a_k , which, while solving the system (1.5.14), turn out to be linear functions of $F(x_k)$. Their substitution into (1.5.13) will show that p_n is also a linear function of $F(x_k)$, that is,

$$p_n(x) = \sum_{k=0}^n l_k(x) F(x_k), \quad (1.5.15)$$

where $l_k(x)$ are polynomials of degree n in $1/(1+x)$ and are known as the *influence functions* of the interpolating points x_k and satisfy the conditions $r_i(x_k) = \delta_{ik}$. Thus,

$$l_k = \prod_{\substack{j=0 \\ j \neq k}}^n \left(\frac{1}{1+x} - \frac{1}{1+x_j} \right) \left[\prod_{\substack{j=0 \\ j \neq k}}^n \left(\frac{1}{1+x_k} - \frac{1}{1+x_j} \right) \right]^{-1}. \quad (1.5.16)$$

The above coefficients $l_k(x)$ differ by very simple factors from the Lagrangian multipliers which, as in (1.5.13), are defined by

$$l_k(x) = \frac{(1+x_k)^n}{(1+x)^n} \frac{\pi_{n+1}(x)}{(x-x_k) \pi'_{n+1}(x_k)},$$

$$\pi_{n+1}(x) = \prod_{j=0}^n (x-x_j). \quad (1.5.17)$$

If we expand the polynomial $\frac{\pi_{n+1}(x)}{(x-x_k)}$ into powers of $1+x$, we get

$$\frac{\pi_{n+1}(x)}{(x-x_k)} = \sum_{m=0}^n c_m^{(k)} (1+x)^m,$$

and after substituting this expansion into (1.5.17) and (1.5.15), we have

$$p_n(x) = \sum_{k=0}^n F(x_k) \sum_{m=0}^n c_m^{(k)} \frac{(1+x_k)^n}{\pi'_{n+1}(x_k)} \frac{1}{(1+x)^{n-m}}, \quad (1.5.18)$$

in which the factors in front of $(1+x)^{-n+m}$ can be computed at the points x_k , $k = 0, 1, \dots, n$. Under the transformation $z = 1/(1+x)$, the error term $E_k(x) = F(x) - p_n(x)$ becomes $e_n(z)$, and is given by

$$\begin{aligned} e_n(z) = & \frac{(-1)^{n+1}}{n!} \int_0^1 G^{(n+1)}(\tau) \left\{ (\tau-z)^n U(\tau-z) \right. \\ & \left. - \sum_{k=0}^n \Lambda_k(z) (\tau-z_k)^n U(\tau-z_k) \right\} d\tau, \end{aligned} \quad (1.5.19)$$

where

$$\Lambda_k(z) = \frac{\pi(z)}{(z-z_k) \pi'(z_k)}, \quad \pi(z) = \prod_{j=0}^n (z-z_j).$$

We can use the inverse transformation to obtain $E_n(x)$ from (1.5.19). Thus, we set $\tau = 1/(1+t)$, $t = 1/\tau - 1$, and after a lengthy calculation (see Krylov and Skoblya 1977, pp. 207–210), we obtain

$$\begin{aligned} E_n(x) = & \int_0^\infty D_{n+1}(F) \frac{1}{n! (1+x)^n} \left[(x-t)^n U(x-t) \right. \\ & \left. - \sum_{k=0}^n \frac{\pi_{n+1}(x)}{(x-x_k) \pi'_{n+1}(x_k)} \frac{(x_k-t)^n}{1+t} U(x_k-t) \right] dt, \end{aligned} \quad (1.5.20)$$

where

$$D_{n+1}(F) = \sum_{j=1}^{n+1} a_{n-j+1} (1+t)^j F^{(j)}(t), \quad a_0 = 1.$$

Note that for $t < x$, x_0, \dots, x_n , the interpolation is exact and the quantity within the braces in (1.5.20) vanishes; otherwise, the functions $U(x-t)$ and $U(x_k-t)$ are equal to zero and the error is also zero. The quantity within the braces in (1.5.20) takes nonzero values only on the interval where x, x_0, \dots, x_n are located. Hence,

in view of the continuity of $D_{n+1}(F)$, the integral over $[0, \infty)$ is a proper definite integral.

1.6. Convergence Accelerators

We discuss some convergence acceleration processes that are useful in quadrature.

1.6.1. Fixed-Point Iteration. To compute the root of an equation $f(x) = 0$, we rearrange $f(x)$ in an equivalent form $x = g(x)$ and use the result that if $f(z) = 0$, where z is a zero of $f(x)$, then $z = g(z)$. The value z is known a *fixed-point* of the function f . Thus, the iterative form

$$x_{n+1} = g(x_n), \quad n = 0, 1, \dots, \quad (1.6.1)$$

converges to the fixed point z of $f(x)$. The fixed-point algorithm is:

Rearrange the equation as an equivalent form $x = g(x)$.

Set $x_2 = x_1$;

REPEAT

 Set $x_1 = x_2$,

 Set $x_2 = g(x_1)$.

UNTIL $|x_1 - x_2| < \text{tolerance}$.

The criterion for the convergence of the sequence $\{x_n\}$ is as follows: If $g \in C^1$ on an interval about a zero z of the equation $x = g(x)$ and if $|g'(x)| < 1$ for all x in the interval, then the sequence $\{x_n\}$ defined by (1.6.1) converges to $x = z$, provided x_i are chosen in the interval.

EXAMPLE 1.6.1. Let $f(x) = x^2 - 2x - 3 = 0$, which has the zeros -1 and 3 . Let a rearrangement be $x = g_1(x) = \sqrt{2x+3}$. If we start with $x = 4$ and iterate with the fixed-point algorithm (1.6.1), we find the successive values as $x_0 = 4$; $x_1 = 3.31662$; $x_2 = 3.10375$; $x_3 = 3.03439$; $x_4 = 3.01144$; $x_5 = 3.00381$; $x_6 = 3.00127$, which appear to be converging to the zero $x = 3$.

If we take the other rearrangement $x = g_2(x) = 3/(x-2)$, and start with $x = 4$, then the fixed-point algorithm yields the following sequence of values: $x_0 = 4$; $x_1 = 1.5$; $x_2 = -6$; $x_3 = -0.375$; $x_4 = -1.26316$; $x_5 = -0.0919355$; $x_6 = -1.02762$; $x_7 = -0.990876$; $x_8 = -1.00305$; $x_9 = -0.998984$; $x_{10} = -1.00034$, which appears to converge to -1 . A third rearrangement is $x = g_3(x) = (x^2 - 3)/2$, and if we start with $x = 4$, the sequence of values is $x_0 = 4$; $x_1 = 6.5$; $x_2 = 19.625$; $x_3 = 191.07$; $x_4 = 18252.4$, and the sequence diverges. This behavior in the three sequences is interesting. Notice that the $|g'(x)|$ is positive but less than 1 in the first case; thus the convergence is monotone. In the second case $|g'(x)|$ is negative and less than 1, and the convergence is oscillatory. In the third case $|g'(x)| > 1$, and the iterates diverge. ■

1.6.2. Aitkin's Δ^2 Process. This is simply a formula that extrapolates the partial sums of a series whose convergence is approximately geometric. In a sequence of values each error is approximately proportional to the previous value. This is the basis for an acceleration technique for convergence. Assume that the three consecutive errors E_n , E_{n+1} and E_{n+2} are defined by $E_i = x_i - r = K^{i-1} E_1$ for $i = n, n+1, n+2$. Then the three successive estimates of the zeros are given by

$$x_i = r + K^{i-1} E_1, \quad i = n, n+1, n+2. \quad (1.6.2)$$

Using this value of x_i we find

$$\frac{x_n x_{n+2} - x_{n+1}^2}{x_{n+2} - 2x_{n+1} + x_n} = r.$$

Thus, from these three successive estimates, we start with x_1 , x_2 and x_3 and extrapolate to an improved estimate. However, the assumption of constant ratio between successive errors is generally not true, and the extrapolated values, though improved, are not exact. An alternative method to avoid the round-off error that occurs in subtracting large numbers of nearly similar magnitude consists in using the forward differences. Thus, define

$$\begin{aligned} \Delta x_i &= x_{i+1} - x_i, \\ \Delta^2 x_i &= \Delta(\Delta x_i) = \Delta(x_{i+1} - x_i) = x_{i+2} - 2x_{i+1} + x_i. \end{aligned}$$

Then Aitkin's acceleration scheme is

$$r = x_n - \frac{(\Delta x_n)^2}{\Delta^2 x_n} = \frac{x_n x_{n+2} - 2x_{n+1}^2}{x_{n+2} - 2x_{n+1} + x_n}. \quad (1.6.3)$$

The criterion to justify when to use Aitkin's acceleration is as follows: Given x_n , x_{n+1} , x_{n+2} , x_{n+3} for some n , compute

$$C = \frac{\sum_{i=n}^{n+2} x_i x_{i+1} - \frac{1}{3} \sum_{i=n}^{n+2} x_i \sum_{i=n}^{n+2} x_{i+1}}{\sqrt{\left[\sum_{i=n}^{n+2} x_i^2 - \frac{1}{3} \left(\sum_{i=n}^{n+2} x_i \right)^2 \right] \left[\sum_{i=n}^{n+2} x_{i+1}^2 - \frac{1}{3} \left(\sum_{i=n}^{n+2} x_{i+1} \right)^2 \right]}}. \quad (1.6.4)$$

Then Aitkin's acceleration is most effective if C is close to unity. Note that Aitken's method can also be used on sequences other than those generated by fixed-point iteration.

EXAMPLE 1.6.2. Consider the same f as in Example 1.6.1. Then $x_{n+1} = \sqrt{2x_n + 3}$. We start with $x_1 = 4$. The extrapolation is given in Table 1.6.2.

Table 1.6.2.

x	Δx	$\Delta^2 x$
$x_1 = 4.000$		
	0.683375	
$x_2 = 3.31662$		0.470498
	0.212877	
$x_3 = 3.10375$		

The accelerated estimate is $r = 4.0 - \frac{(0.683375)^2}{0.470498} = 3.00743$. Using the value of $x_0 = 4$, $x_1 = 3.31662$, $x_2 = 3.10375$, and $x_3 = 3.03439$, we find that

$$C = \frac{32.9764 - \frac{1}{3}(10.4204)(9.45476)}{\sqrt{(36.6332 - 36.1847)(29.8408 - 29.7975)}} = 0.973095.$$

See Jones (1982) for other extensions to improve the acceleration technique.

Alternatively, we define Aitken's Δ^2 -algorithm as follows: Given a sequence $\{x_0, x_1, x_2, \dots\}$ that converges to ξ , compute the sequence $\{\hat{x}_1, \hat{x}_2, \dots\}$ by the formula $\hat{x}_n = x_{n+1} - \frac{(\Delta x_n)^2}{\Delta^2 x_{n-1}}$. This is known as Aitkin's Δ^2 process; it is applicable to any linearly convergent sequence.

If the sequence $\{x_0, x_1, x_2, \dots\}$ converges linearly to ξ , i.e., if the error $\xi - x_{n+1} = K(\xi - x_n) + o(\xi - x_n)$ for some $K \neq 0$, then $\hat{x}_n = \xi - o(\xi - x_n)$. Also, if from certain k onward, the sequence of difference ratios $\left\{ \frac{\Delta x_k}{\Delta x_{k-1}}, \frac{\Delta x_{k+1}}{\Delta x_k}, \dots \right\}$ is almost constant, then \hat{x}_k can be taken as a better approximation to ξ than x_k . In particular, $|\hat{x}_k - x_k|$ then becomes a good estimate for the error $|\xi - x_k|$. If we reach a certain \hat{x}_k which we decide as a much better approximation to ξ than x_k , then the process stops, and we start the fixed-point iteration with \hat{x}_k as an initial guess by using the *Steffensen's iteration* which is defined by

STEFFENSEN'S ALGORITHM. Given the iteration function $g(x)$ and a point y_0 ,

For $n = 0, 1, 2, \dots$, until satisfied, do

Set $x_0 = y_n$

Compute $x_1 = g(x_0)$, $x_2 = g(x_1)$

Compute $d = \Delta x_1$, $r^{-1} = \Delta x_0/d$

Compute $y_{n+1} = x_2 + d/(r^{-1} - 1)$

enddo

A Fortran program for this algorithm is provided as `aitken.f90` on the CD-R.

The Steffensen's algorithm is combined with an ordinary fixed-point iteration as follows: Initially, we use fixed-point iteration to generate the iterates x_0, x_1, x_2, \dots , and also to compute the ratios $r_1^{-1}, r_2^{-1}, \dots$. When these ratios become sufficiently constant, we switch over to Steffensen's iteration. The program terminates if $v > \text{ntol}$ or $|g(x_n) - x_n| \leq \text{xtol}$, where ntol denotes the upper bound on the number of steps to be carried out and xtol is a given absolute-error requirement.

1.6.3. Shanks Process. Shanks (1955) uses the idea of fitting the elements A_r of a sequence $\{A_r\}$, $r = 0, 1, 2, \dots$, to a predefined form which has free constants, and then computing these constants, such that the limit of the predefined form yields the estimate of the required limit. The sequence of the estimated limits itself forms a sequence, which should converge faster than the original sequence to the same limit. Shanks uses the predefined form

$$A_r = B_{kn} + \sum_{i=1}^k \alpha_{ik} q_{in}^r, \quad q_{in} \neq 1 \text{ or } 0, \text{ for } n-k \leq r \leq n+k, \text{ and } n \geq k, \quad (1.6.5)$$

where the term B_{kn} is known as the *local base*. It is obvious that B_{kn} approaches the required limit as $r \rightarrow \infty$. Hence, there are $2k+1$ nonlinear equations for the free constants B_{kn} , α_{in} and q_{in} , and we are required to compute B_{kn} .

However, these nonlinear equations can be solved by using the following results: If the quantities p_s are defined by $p_s = \sum_{i=1}^k a_i q_i^s$, $s = 0, 1, \dots, 2k-1$, then q_i are the roots of the equation

$$\begin{vmatrix} 1 & q & \cdots & q^{k-1} & q^k \\ p_0 & p_1 & \cdots & p_{k-1} & p_k \\ p_1 & p_2 & \cdots & p_k & p_{k+1} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ p_{k-1} & p_k & \cdots & p_{2k-2} & p_{2k-1} \end{vmatrix} = 0. \quad (1.6.6)$$

Thus, by taking the forward differences of successive equations in (1.6.5), and replacing p_s by ΔA_{n-k+s} and a_i by $\alpha_{in} |q_{ik}^{n-k+1} - q_{in}^{n-k}|$, we find from (1.6.6) that q_n are the roots of the equation

$$\begin{vmatrix} 1 & q & \cdots & q^k \\ \Delta A_{n-k} & \Delta A_{n-k+1} & \cdots & \Delta A_n \\ \vdots & \vdots & \cdots & \vdots \\ \Delta A_{n-1} & \Delta A_n & \cdots & \Delta A_{n+k-1} \end{vmatrix} = 0,$$

or

$$c_n q^k + c_{n-1} q^{n-1} + \cdots + c_{n-k} = 0, \quad (1.6.7)$$

where c_j denotes the minors obtained by expanding the determinant on the left side of (1.6.7) by its first row. If we substitute the expansion for A_j from (1.6.5) into the

expression

$$\frac{c_{n-k} A_{n-k} + \dots + c_{n-1} A_{n-1} + c_n A_n}{c_n - k} + \dots + c_{n-1} + c_n,$$

which is the expansion by its first row of the ratio

$$\frac{\begin{vmatrix} A_{n-k} & \cdots & A_{n-1} & A_n \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \Delta A_{n-k+1} & \cdots & \Delta A_n & \Delta A_{n+1} \\ \vdots & \cdots & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & \Delta A_{n-k-2} & \Delta A_{n+k-1} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 & 1 \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \Delta A_{n-k+1} & \cdots & \Delta A_n & \Delta A_{n+1} \\ \vdots & \cdots & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & \Delta A_{n-k-2} & \Delta A_{n+k-1} \end{vmatrix}} = B_{nk}. \quad (1.6.8)$$

Some simple cases of this process are:

CASE 1. With determinants of order 2 (i.e., $k = 1$), we obtain from (1.6.8) the well-known *Aitken's extrapolation formula*

$$B_{1k} = \frac{A_{n-1}A_{n+1} - A_n^2}{A_{n+1} - 2A_n + A_{n-1}}, \quad (1.6.9)$$

which can be applied to successive sequences of three terms and generates a new sequence $\{B_{1n}, B_{2n} \dots\}$, often denoted by the *operator* e_1 , where

$$e_1(A) = \{B_{1n}\}, \quad n \geq 1. \quad (1.6.10a)$$

The general form of this operator is e_k which is defined by

$$e_k(A) = \{B_{kn}\}, \quad n \geq k. \quad (1.6.10b)$$

Another operator, known as the *diagonal operator* e_d , is defined by

$$e_d(a) = \{B_{nn}\}. \quad (1.6.10c)$$

These operators are used to generate a table of new sequences, in which the first column is the original sequence, the second is e_1 , the third e_2 , and so on; the operator e_d then appears at the top of the table, which is known as the *Shanks table* and can be extended until the desired convergence is achieved. Alternatively, we can use simple transformation repeatedly by applying e_1 to the second column to get the third, thus obtaining columns with the transformations e_1, e_1^2 , and so on (see [Example 1.6.3](#)).

EXAMPLE 1.6.3. Consider the coefficients A_n in the Taylor’s series for $\ln(1+x)$:

$$A_n = \sum_{j=1}^n \frac{(-1)^{j+1}2^j}{j}.$$

The results of the above transformation are given in Table 1.6.3, which exhibits the rapid convergence to the limit value of $\ln 3 \approx 1.0986122886$.

Table 1.6.3.

k	A_k	e_d
1	2.0	
2	0.0	1.142857
3	2.66667	1.114492
4	-1.33333	1.0988056
5	5.066667	1.0986256
6	-5.6	1.09861323

1.6.4. ϵ -Algorithm. The use of ϵ -algorithm (Wynn 1956) with the Shanks accelerators makes the process very effective. The ϵ -algorithm uses the recurrence relations

$$\begin{aligned} \epsilon_0^{-1} &= 0, \\ \epsilon_n^0 &= A_n, \\ \epsilon_n^{(p)} &= \epsilon_{n+1}^{(p-2)} + \left[\epsilon_{n+1}^{(p-1)} - \epsilon_n^{(p-1)} \right]^{-1}. \end{aligned} \tag{1.6.11}$$

Then in terms of these ϵ -values the accelerated sequences are given by $B_{kn} = \epsilon_{n-k}^{(2k)}$, which yields a table of the form

$\epsilon_0^{(-1)}$					
$\epsilon_1^{(-1)}$	$\epsilon_0^{(0)}$				
$\epsilon_2^{(-1)}$	$\epsilon_1^{(0)}$	$\epsilon_0^{(1)}$			
$\epsilon_3^{(-1)}$	$\epsilon_2^{(0)}$	$\epsilon_1^{(1)}$	$\epsilon_0^{(2)}$		
$\epsilon_4^{(-1)}$	$\epsilon_3^{(0)}$	$\epsilon_2^{(1)}$	$\epsilon_1^{(2)}$	$\epsilon_0^{(3)}$	
$\epsilon_5^{(-1)}$	$\epsilon_4^{(0)}$	$\epsilon_3^{(1)}$	$\epsilon_2^{(2)}$	$\epsilon_1^{(3)}$	$\epsilon_0^{(4)}$
	$\{A_n\}$		$\{B_{1n}\}$		$\{B_{2n}\}$

where the columns for the sequences $\{A_n\}$, $\{B_{1n}\}$ and $\{B_{2n}\}$ are marked in the last row. This table is constructed by taking the first three A -values and the values of $\epsilon_0^{(2)}$ are found. Then two more A -values are added and the table is completed through

$\epsilon_0^{(4)}$. Depending on the desired convergence, the process is continued row by row, until a suitable agreement is found in the new sequence, at which time the process is terminated. For details of this and other transforms, see [algorithms.pdf](#) on the CD-R.

1.6.5. Levin's Transformation. In some cases the predetermined form (1.6.5) fails to be generated in the Shanks process; an example is $A_r = 1/r^2$. Levin (1973) improved upon the Shanks transformation by assuming that

$$A_r = T_{kn} + R_r \sum_{i=0}^{k-1} \gamma_{in} f_i(r), \quad n \leq r \leq n+k, \quad (1.6.12)$$

where γ_{in} are free to force the fit to the given sequence, and R_r and $f_i(r)$ are chosen to provide a range of different methods. Thus, Eqs (1.6.12) form a system of linear algebraic equations which yield

$$T_{kn} = \frac{\begin{vmatrix} A_n & A_{n+1} & \cdots & A_{n+k} \\ R_n f_0(n) & R_{n+1} f_0(n+1) & \cdots & R_{n+k} f_0(n+k) \\ R_n f_1(n) & R_{n+1} f_1(n+1) & \cdots & R_{n+k} f_1(n+k) \\ \vdots & \cdots & \vdots & \vdots \\ R_n f_{k-1}(n) & R_{n+1} f_{k-1}(n+1) & \cdots & R_{n+k} f_{k-1}(n+k) \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \cdots & 1 \\ R_n f_0(n) & R_{n+1} f_0(n+1) & \cdots & R_{n+k} f_0(n+k) \\ R_n f_1(n) & R_{n+1} f_1(n+1) & \cdots & R_{n+k} f_1(n+k) \\ \vdots & \cdots & \vdots & \vdots \\ R_n f_{k-1}(n) & R_{n+1} f_{k-1}(n+1) & \cdots & R_{n+k} f_{k-1}(n+k) \end{vmatrix}}.$$

If we take $f_i(r) = r^{-i}$ and divide successive columns by $R_n, R_{n+1}, \dots, R_{n+k}$ and the expansion by the first row, we get

$$T_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{A_{n+j}}{R_{n+j}}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{1}{R_{n+j}}}. \quad (1.6.13)$$

1.6.6. t -Transformation. This transformation is obtained if we set $R_r = a_r = \Delta A_{r-1}$ in (1.6.12). This yields the operators t_k and t_d , which are defined analogous to e_k and e_d , by

$$t_k(A) = \{T_{kn}\}, \quad t_d(A) = \{T_{n1}\}. \quad (1.6.14)$$

There are two modifications of the t -transformation, depending on the following two

different choices of R_r : (i) If $R_r = r a_r$, we get the u -transformation with the formula

$$U_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{A_{n+j}}{R_{n+j}}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{1}{a_{n+j}}}, \quad (1.6.15)$$

with the corresponding operators

$$u_k(A) = \{U_{kn}\}, \quad u_d(A) = \{U_{n1}\}.$$

(ii) This is the Shanks transformation of the t -transform, which is obtained by writing the Aitken extrapolation rule (1.6.9) as

$$e_1(A)_n = \frac{A_{n-1} a_{n+1} - A_n a_n}{a_{n+1} - a_n} = A_n + \frac{a_n a_{n+1}}{a_n - a_{n+1}},$$

which, by taking $R_r = a_r a_{r+1} / (a_{r+1} - a_r)$, leads to the v -transformation defined by

$$V_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{a_{n+j-1} - a_{n+j}}{a_{n+j} a_{n+j+1}} A_{n+j}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} \frac{a_{n+j-1} - a_{n+j}}{a_{n+j} a_{n+j+1}}}, \quad (1.6.16)$$

with the corresponding operators

$$v_k(A) = \{V_{kn}\}, \quad v_d(A) = \{V_{n1}\}.$$

The transformation discussed in this section are very useful in quadrature, especially in accelerating the sequences of computed values to ensure better convergence.

1.6.7. D - and W -Transformations. (Sidi 1987, pp. 349-351) The D -transformation was analyzed by Sidi (1979) for its convergence properties using Richardson's extrapolation process. Two modifications of the D -transformations were proposed by Sidi (1980); they are known as \bar{D} - and \tilde{D} -transformations. They are useful in simplifying the computation of oscillatory infinite integrals, with emphasis on the Fourier and Hankel transforms where the integrands involve a sine or a cosine, or a combination of both, of the integration variable (see Sidi 1980b). Levin and Sidi (1981) proposed a nonlinear extrapolation method for accelerating the convergence of infinite integrals of the form $I_a^\infty(f)$, $a \geq 0$. Another modification, known as the W -transformation, is available in Sidi (1982) and is very useful in dealing with 'very oscillatory' infinite integrals (see Chapter 4), a modification of this W -transformation is found in Sidi (1987, 1988) and this is useful in dealing with divergent infinite integrals, with detailed convergence analysis. The value of these modifications of

the D -transformation lies in their ability to achieve a prescribed accuracy level with considerably less computation.

We assume that the integral $I_a^\infty - \int_a^x = I_x^\infty(f)$ has a well-defined asymptotic expansion as $x \rightarrow \infty$. Thus, as shown by examples in Levin and Sidi (1981), a very large family of functions $f(t)$ that are not singular at infinity, possess asymptotic expansions of the form

$$\begin{aligned} \int_a^\infty f(t) dt - \int_a^x f(t) dt &= \int_x^\infty f(t) dt \\ &\sim \sum_{k=0}^{m-1} x^{\rho_k} f^{(k)}(x) \sum_{i=0}^{\infty} \tilde{\beta}_{ki} x^{-i} \quad \text{as } x \rightarrow \infty, \end{aligned} \quad (1.6.17)$$

where $\rho_k \leq k+1$ are some integers that depend on $f(x)$, and $\tilde{\beta}_{ki}$ are coefficients that are independent of x . Once it is established that an asymptotic expansion of the type (1.6.17) exists, the integral $\int_a^\infty f(t) dt$ can be determined by using the D -transformation as follows: Choose a sequence of nodes $a < x_0 < x_1 < \dots$, such that $\lim_{i \rightarrow \infty} x_i = \infty$; then compute the finite integrals $\int_a^{x_i} f(t) dt$, $i = 0, 1, 2, \dots$, by using the appropriate quadrature formula. For given nonnegative integers j and n_k , $k = 0, 1, \dots, m-1$, define the approximation $D_n^{(m,j)}$, where $N \equiv (n_0, n_1, \dots, n_{m-1})$, as the solution of the system of linear equations

$$D_n^{(m,j)} - \int_a^{x_p} f(t) dt = \sum_{k=0}^{m-1} x_p^{\rho_k} f^{(k)}(x_p) \sum_{i=0}^{n_k} \beta_{ki} x_p^{-i}, \quad j \leq p \leq j + N, \quad (1.6.18)$$

where $N = \sum_{k=0}^{m-1} (n_k + 1)$, and β_{ki} are the remaining N unknowns. The D -transformation can be simplified by replacing ρ_k in (1.6.18) by $(k+1)$ for $0 \leq k \leq m-1$ (Sidi 1990), and it will not seriously affect the accuracy. The solution of the system (1.6.18) for $D_n^{(m,j)}$ can be obtained recursively by using the W -algorithm for $m = 1$ (Sidi 1982), and by the $W^{(m)}$ -algorithm for $m > 1$ (see Ford and Sidi 1987; also §5.3.3 for Levin's transformation).

1.7. Polynomial Splines

A polynomial spline of degree n is a piecewise polynomial of the same degree with continuous $(n-1)$ -th derivatives. A spline of degree n with $(N+1)$ knots x_k , $k = 0, 1, \dots, N$, is of the form

$$\sum_{k=0}^n \alpha_k x^k + \sum_{k=0}^N \beta_k (x - x_k)_+^n, \quad (1.7.1)$$

where

$$z_+ = \begin{cases} z & \text{if } z \geq 0, \\ 0 & \text{if } z < 0, \end{cases}, \quad \text{and } z_+^0 = 1 \text{ only if } z \geq 0.$$

According to Rice (1983), splines of the form (1.7.1) are not always suitable for computation. A spline fits a polynomial to a set of data. A cubic spline fits a “smooth curve” to the data points; it is known as a *French curve* in the drafting jargon. A cubic spline in the i -th interval, which lies between the points (x_i, y_i) and (x_{i+1}, y_{i+1}) , has the equation

$$g_i(x) = a_i (x - x_i)^3 + b_i (x - x_i)^2 + c_i (x - x_i) + d_i. \quad (1.7.2)$$

We seek a cubic spline function $f(x)$ which is such that $g(x) = g(x_i)$ on the interval $[x_i, x_{i+1}]$ for $i = 0, 1, \dots, n-1$, and satisfies the conditions

$$\begin{aligned} g_i(x_i) &= y_i, \quad i = 0, 1, \dots, n-1, \quad \text{and } g_{n-1}(x_n) = y_n, \\ g_i(x_{i+1}) &= g_{i+1}(x_{i+1}) = g_{i+1}(x_{i+1}) \quad \text{for } i = 0, 1, \dots, n-2, \\ g'_i(x_{i+1}) &= g'_{i+1}(x_{i+1}) \quad \text{for } i = 0, 1, \dots, n-2, \\ g''_i(x_{i+1}) &= g''_{i+1}(x_{i+1}) \quad \text{for } i = 0, 1, \dots, n-2. \end{aligned} \quad (1.7.3)$$

There are $4n$ unknowns $\{a_i, b_i, c_i, d_i\}$ for $i = 0, 1, \dots, n-1$. Solving (1.7.2)–(1.7.3), we obtain the recurrence relation

$$\begin{aligned} h_{i-1} S_{i-1} + (2h_{i-1} + 2h_i) S_i + h_i S_{i+1} \\ = 6\{f[x_i, x_{i+1}] - f[x_{i-1}, x_i]\}, \end{aligned} \quad (1.7.4)$$

where $h_i = x_{i+1} - x_i$, $S_i = g''_i(x_i)$ for $i = 0, 1, \dots, n-1$, and $S_n = g''_{n-1}(x_n)$. Eq (1.7.4) applies to all $n-1$ interior points from $i = 1$ to $i = n-1$, thus giving $n-1$ equations for the $n+1$ values of S_i ; the two remaining equations for S_0 and S_n are obtained from the conditions at the two endpoints of the interval. However, these two conditions are arbitrary but they are chosen from the following choices:

1. Take $S_0 = 0$ and $S_n = 0$. Thus, the end cubics approach linearity at their endpoints. This condition is known as the *natural spline* and, although it flattens the curve too much at the ends, it is used frequently.

2. Make the slopes at the endpoints assume specific values. If the slopes are not precisely known, they might be estimated from the points. For example, if $f'(x_0) = A$ and $f'(x_n) = B$, we use the divided differences and use the relations

$$\begin{aligned} \text{At left endpoint:} \quad 2h_0 S_0 + h_1 S_1 &= 6(f[x_0, x_1] - A), \\ \text{At right endpoint:} \quad h_{n-1} S_{n-1} + 2h_n S_n &= 6(B - f[x_{n-1}, x_n]). \end{aligned}$$

This seems to be the best choice, provided reasonable estimates of the derivative are available.

3. Take $S_0 = S_1$, and $S_{n-1} = S_n$, so that the end cubics approach parabolas at their endpoints.

4. Take S_0 as a linear extrapolation from S_1 and S_2 , and S_n as a linear extrapolation from S_{n-1} and S_{n-2} . This makes the cubic splines match $f(x)$ exactly when $f(x)$ is itself a cubic curve. For this choice we use the following relations:

$$\begin{aligned} \text{At left endpoint: } \quad \frac{S_1 - S_0}{h_0} &= \frac{S_2 - S_1}{h_1} \Rightarrow S_0 = \frac{(h_0 + h_1) S_1 - h_0 S_2}{h_1}, \\ \text{At right endpoint: } \quad \frac{S_n - S_{n-1}}{h_{n-1}} &= \frac{S_{n-1} - S_{n-2}}{h_{n-2}} \\ &\Rightarrow S_n = \frac{(h_{n-2} + h_{n-1}) S_{n-1} - h_{n-1} S_{n-2}}{h_{n-2}}. \end{aligned}$$

This choice gives too much curvature in the end intervals.

The details of these choices are as follows. Eq (1.7.4) which solves for S_i , $i = 0, 1, \dots, n$, can be written in matrix form as

$$\begin{bmatrix} h_0 & 2(h_0 + h_1) & h_1 & & & \\ & h_1 & 2(h_1 + h_2) & h_2 & & \\ & & h_2 & 2(h_2 + h_3) & h_3 & \\ & & & \ddots & & \\ & & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) & h_{n-1} \end{bmatrix} \begin{Bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \\ \vdots \\ S_{n-1} \\ S_n \end{Bmatrix} = 6 \begin{Bmatrix} f[x_1, x_2] - f[x_0, x_1] \\ f[x_2, x_3] - f[x_1, x_2] \\ f[x_3, x_4] - f[x_2, x_3] \\ \vdots \\ f[x_{n-1}, x_n] - f[x_{n-2}, x_{n-1}] \end{Bmatrix}.$$

Note that in this matrix equation the first and the last rows are missing; they correspond to S_0 and S_n . Now, we start with each of the above choices, and write the form of the left-side matrix in each case.

CHOICE 1. $S_0 = 0 = S_n$, and

$$\begin{bmatrix} 2(h_0 + h_1) & h_1 & & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & & \\ & h_2 & 2(h_2 + h_3) & h_3 & & \\ & & & \ddots & & \\ & & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) \end{bmatrix}.$$

CHOICE 2. $f'(c_0) = A$ and $f'(x_n) = B$, and

$$\begin{bmatrix} 2h_0 & h_1 & & & \\ h_1 & 2(h_0 + h_1) & h_1 & & \\ & h_1 & 2(h_1 + h_2) & h_2 & \\ & & & \vdots & \\ & & & h_{n-2} & 2h_{n-1} \end{bmatrix}.$$

CHOICE 3. $S_0 = S_1$, $S_n = S_{n-1}$, and

$$\begin{bmatrix} (3h_0 + 2h_1) & h_1 & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & \\ & h_2 & 2(h_2 + h_3) & h_3 & \\ & & & \vdots & \\ & & & h_{n-2} & (2h_{n-2} + 3h_{n-1}) \end{bmatrix}.$$

CHOICE 4. S_0 and S_n are linear extrapolations, and

$$\begin{bmatrix} H_0 & \frac{h_1^2 - h_0^2}{h_1} & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & \\ & h_2 & 2(h_2 + h_3) & h_3 & \\ & & & \vdots & \\ & & & \frac{h_{n-2}^2 - h_{n-1}^2}{h_{n-2}} & H_n \end{bmatrix},$$

where

$$H_0 = \frac{(h_0 + h_1)(h_0 + 2h_1)}{h_1}, \quad H_n = \frac{(h_{n-1} + h_{n-2})(h_{n-1} + 2h_{n-2})}{h_{n-2}}.$$

After computing the values of S_i , the coefficients in (1.7.4) are given by

$$a_i = \frac{S_{i+1} - S_i}{6h_i}, \quad b_i = \frac{S_i}{2}, \quad c_i = \frac{y_{i+1} - y_i}{h_i} - \frac{2h_i S_i + h_i S_{i+1}}{6}, \quad d_i = y_i = f(x_i). \quad (1.7.5)$$

If $f(x)$ is periodic and the data cover one full period, then a choice is to take $S_0 = S_n$ and equal slopes at the two endpoints.

EXAMPLE 1.7.1. Consider a data

$$\mathbf{d} = \{f(0), f(1), f(1.7), f(2.6)\} = \{2, 4.43656, 8.05789, 20.16747\}.$$

Use cubic splines to compute $f(0.76)$ and $f(1.35)$. Here, $h_0 = 1$, $h_1 = 0.7$, and $h_2 = 0.8$; the divided differences are $f[0, 1] = 2.43656$, $f[1, 1.7] = 5.17333$,

$f[1.7, 2.6] = 13.4551$. For a natural cubic spline, we use the end condition 1 with $S_0 = 0 = S_3$, and solve

$$\begin{bmatrix} 2(h_0 + h_1) & h_1 \\ h_1 & 2(h_1 + h_2) \end{bmatrix} \begin{Bmatrix} S_1 \\ S_2 \end{Bmatrix} = 6 \begin{Bmatrix} f[0, 1] - f[1, 1.7] \\ f[1.7, 2.6] - f[1, 1.7] \end{Bmatrix},$$

which becomes

$$\begin{bmatrix} 3.4 & 0.7 \\ 0.7 & 3.2 \end{bmatrix} \begin{Bmatrix} S_1 \\ S_2 \end{Bmatrix} = \begin{Bmatrix} 16.4206 \\ 49.6906 \end{Bmatrix},$$

and yields $S_1 = 1.70958$ and $S_2 = 15.1543$. The values of a_i , b_i , c_i and d_i are

$$\begin{aligned} a_i &= \{0.28493, 3.20112, -2.80635\}, & b_i &= \{0, 0.85479, 7.67715\}, \\ c_i &= \{2.15613, 3.00643, 8.9088\}, & d_i &= \{2, 4.435556, 8.05789\}. \end{aligned}$$

Thus, $g_i(x)$, defined by (1.7.2), approximates $f(x)$. Using the above values we find that $f(0.76) \approx g_1(0.76) = 3.76032$, and $f(1.35) \approx g_2(1.35) = 5.73077$. The exact function is $f(x) = 2e^x - x^2$, which gives the exact values as $f(x) = 3.69895$ and $f(1.35) = 5.89235$. ■

2

Interpolatory Quadrature

We start with the basic concepts of Riemann integration and present numerical method for evaluating certain integrals by replacing the integrands by approximating functions, develop the method of the Riemann sums, and discuss interpolatory quadrature rules for computing the definite integral $I_a^b(f) \equiv \int_a^b f(x) dx$. We discuss interpolatory quadrature formulas in their basic and repeated (extended or compound) forms, and some of the extensions which are known as the Romberg's and Gregory's schemes. We also present quadrature rules which use nodes outside the interval of integration. The error bounds for all quadrature rules are presented, and some iterative and adaptive schemes are analyzed.

2.1. Riemann Integration

Riemann integrals of a function $f(x) \in C[a, b]$ on an interval $[a, b]$, denoted by

$$I_a^b(f) = \int_a^b f(x) dx, \quad (2.1.1)$$

are defined in terms of the Riemann sum as follows. Let $\mathcal{P} = \{x_0, x_1, \dots, x_n\}$ be any partition of $[a, b]$. For each k , where $1 \leq k \leq n$, let ξ_k be an arbitrary point in $[x_{k-1}, x_k]$, and let $\Delta x_k = |x_k - x_{k-1}|$ denote the length of each subinterval for $k = 1, 2, \dots, n$. Then the sum

$$R_n f = \sum_{k=1}^n f(\xi_k) \Delta x_k, \quad (2.1.2)$$

is called the *Riemann sum* for f on $[a, b]$. Let $\|\mathcal{P}\|$ denote the norm of the partition \mathcal{P} ; i.e., it is the largest of the lengths of the subintervals associated with \mathcal{P} . Then

$$\lim_{\|\mathcal{P}\| \rightarrow 0} \sum_{k=1}^n f(\xi_k) \Delta x_k = I_a^b(f). \quad (2.1.3)$$

This convergence of the Riemann sum to $I_a^b(f)$ can also be defined as follows: For any $\varepsilon > 0$ there is a number $\delta > 0$ such that if each of the subintervals $[x_{k-1}, x_k]$ has length less than δ and if $x_{k-1} \leq \xi_k \leq x_k$ for $1 \leq k \leq n$, then

$$\left| I_a^b(f) - \sum_{k=1}^n f(\xi_k) \Delta x_k \right| < \varepsilon. \quad (2.1.4)$$

The indefinite integration is defined in terms of the relation between the antiderivatives and integrals, and the notation traditionally used for an antiderivative of f is $\int f(x) dx$, which is called an *indefinite integral*. Thus,

$$\int f(x) dx = F(x) \quad \text{means} \quad F'(x) = f(x). \quad (2.1.5)$$

In general, this definition is generalized to

$$\int f(x) dx = F(x) + C \quad \text{is equivalent to} \quad \frac{d}{dx} \{F(x) + C\} = f(x), \quad (2.1.6)$$

where C is an arbitrary constant, known as the *constant of integration*. Thus, the indefinite integral $\int f(x) dx$ implies either a particular antiderivative of f or an entire family of antiderivatives, one for each value of the constant C . Care is needed to distinguish between definite and indefinite integrals. A definite integral $I_a^b(f) = \int_a^b f(x) dx$ is a number, whereas an indefinite integral $\int f(x) dx$ is a function of x .

Tables of indefinite integrals are sometimes very useful when we run into an indefinite integral which is difficult to evaluate by hand and we do not have access to computer algebra systems, like Mathematica, and others. An extensive table of formulas for indefinite and definite integrals is provided on the enclosed CD-R, §8, titled ‘Integration Formulas.’

2.1.1. Approximate Integration. There are different methods for computing approximate solutions of definite integrals $I_a^b(f)$. Most of these methods are derived from interpolating polynomials and orthogonal polynomials and will be discussed in following sections. We use three methods to approximate the definite integrals $I_a^b(f)$.

METHOD 1: RIEMANN SUMS. We will use formula (2.1.2) by considering the n subintervals of $[a, b]$ which are of equal length. Then $x_k = a + kh$, $k = 0, 1, \dots, n$,

where $h = (b - a)/n$ is known as the *step size*. We choose the point ξ_k as the left or right endpoint of the subinterval $[x_{k-1}, x_k]$. If $\xi_k = x_{k-1}$, then we have $R_n^l f = h \sum_{k=1}^n f(x_{k-1})$; or, if $\xi_k = x_k$, we have $R_n^r f = h \sum_{k=1}^n f(x_k)$, where the superscript l or r designates the left or right endpoint of the interval $[x_{k-1}, x_k]$ chosen. It is easy to show that each $R_n^l f$ and $R_n^r f$ converges to $I_a^b(f)$ as $n \rightarrow \infty$ for any Riemann-integrable function f . If $f \in C[a, b]$, then the (discretization) error bound is given by

$$|I_a^b(f) - R_n f| \leq (b - a) \omega(f; h), \tag{2.1.7}$$

where $\omega(f; h)$ is the modulus of continuity of f .

EXAMPLE 2.1.1. Consider the following integrands: (i) $f_1(x) = x^2$, (ii) $f_2(x) = \sin \pi x$, and (iii) $f_3(x) = \sqrt{x}$, each with the interval of integration $[0, 1]$. The results of the approximate values of $I_0^1(f_i)(x)$, $i = 1, 2, 3$, are presented in Table 2.1.1. It is obvious that the convergence of this method is extremely slow. ■

Table 2.1.1

n	$R_n f_1$	$R_n f_2$	$R_n f_3$
4	0.4687 50000	0.6035 53390	0.7682 83046
16	0.3652 34375	0.6345 73149	0.6948 31196
64	0.3411 86523	0.6364 91935	0.6740 83211
256	0.3352 89001	0.6366 11786	0.6685 69673
1024	0.3338 21773	0.6366 19273	0.6671 48643
4096	0.3334 55413	0.6366 19741	0.6667 87946
Exact	0.3333 33333	0.6366 19772	0.6666 66666

METHOD 2: APPROXIMATING FUNCTIONS. In some cases we can use an approximating function to compute an approximate solution for $I_a^b(f)$. Let a function g approximate f on $[a, b]$ such that $\|g - f\|_\infty \leq \varepsilon/(b - a)$, where $\varepsilon > 0$ is arbitrary. Then the error bound is

$$\begin{aligned} \|I_a^b(f) - I_a^b(g)\| &= \left| \int_a^b f(x) dx - \int_a^b g(x) dx \right| \\ &= \int_a^b |f(x) - g(x)| dx \leq (b - a) \|f - g\|_\infty \leq \varepsilon. \end{aligned} \tag{2.1.8}$$

EXAMPLE 2.1.2. Compute $\int_0^1 \sqrt{x} \Gamma(x + 1) dx$ by using the approximation (Abramowitz and Stegun 1968, p. 257)

$$\Gamma(x + 1) = 1 + \sum_{k=1}^8 b_k x^k + E_8(x), \quad |E_8(x)| \leq 3 \times 10^{-7},$$

where

$$\begin{aligned} b_1 &= -0.57719\,1652, & b_5 &= -0.756704078, \\ b_2 &= 0.98820\,5891, & b_6 &= 0.48219\,9394, \\ b_3 &= -0.89705\,6937, & b_7 &= -0.19352\,7818, \\ b_4 &= 0.91820\,6857, & b_8 &= 0.03586\,8343. \end{aligned}$$

The computed value is $I = 0.614620138422$, which compares well with the Mathematica value of 0.6145201406413421 . ■

METHOD 3: TAYLOR SERIES METHOD. Consider the function $f \in C^\infty[-1, 1]$. If both $x, a \in [-1, 1]$, the Taylor series expansion at $x = a$ is

$$f(x) = f(a) + (x-a)f'(a) + \cdots + \frac{(x-a)^{n-1}}{(n-1)!} f^{(n-1)}(a) + \int_a^x \frac{(x-t)^{n-1}}{(n-1)!} f^{(n)}(t) dt.$$

Without loss of generality, we take $a = 0$. Then

$$\begin{aligned} I_{-1}^1(f) &= 2f(0) + \frac{2}{3}f''(0) + \cdots + \frac{1 - (-1)^n}{n!} f^{(n-1)}(0) + I(E_n f), \\ Q_n(f) &= f(0) \sum_{i=1}^n + f'(0) \sum_{i=1}^n A_i x_i + \frac{f''(0)}{2!} \sum_{i=1}^n A_i x_i^2 + \cdots \\ &\quad + \frac{f^{(n-1)}(0)}{(n-1)!} \sum_{i=1}^n A_i x_i^{n-1} + Q_n(E_n f), \end{aligned} \quad (2.1.9)$$

where $E_n f = \int_0^x \frac{(x-t)^{n-1}}{(n-1)!} f^{(n)}(t) dt$. Neglecting $I(E_n f)$ and $Q_n(E_n f)$, and comparing the corresponding terms in $I_{-1}^1(f)$ and $Q_n(f)$, we obtain from (2.1.9)

$$\sum_{i=1}^n A_i x_i^k = \frac{1 - (-1)^n}{k+1}, \quad k = 0, 1, \dots, n-1. \quad (2.1.10)$$

Eq (2.1.10), known as the *momentum equations*, represents a linear system in the n unknown weights A_i . Using the Vandermonde matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ x_1^2 & x_2^2 & \cdots & x_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{bmatrix}, \quad (2.1.11)$$

we find that for distinct nodes x_i

$$\det(\mathbf{A}) = \prod_{k=2}^n \prod_{j=1}^{k-1} (x_k - x_j) \neq 0. \quad (2.1.12)$$

It is not necessary that all x_i be in $[-1, 1]$. Formula (2.1.12) is also valid for nodes x_i that are outside the interval $[-1, 1]$ provided the Taylor expansion is valid there. The first equation in (2.1.11) is

$$\sum_{i=1}^n A_i = 2 \quad \text{for } w(x) \neq 1, \text{ where } \int_{-1}^1 w(x) dx = \sum_{i=1}^n A_i. \quad (2.1.13)$$

It means that the sum of the weights is equal to the area of the domain of integration.

EXAMPLE 2.1.3. The weights of $Q_3 f = A_1 f(-1) + A_2 f(0) + A_3 f(1)$ are determined by solving the equations (2.1.11), which are $A_1 + 1 + A_2 + A_3 = 2$, $-A_1 + A_3 = 0$, and $A_1 + A_3 = 2/3$, which are solved to give $A_1 = A_3 = 1/3$ and $A_2 = 4/3$. Hence,

$$Q_3 f = \frac{1}{3} [f(-1) + 4f(0) + f(1)],$$

which is the Simpson's rule,* discussed in §2.5. ■

If instead of the fixed nodes x_i which are preassigned numbers or vectors we treat the nodes as n additional unknown quantities, we end up with a system of $2n$ equations in $2n$ unknowns x_i and A_i , $i = 1, 2, \dots, n$, which is known as the *enlarged system of momentum equations* defined by

$$\sum_{i=1}^n A_i x_i^k = I(x^k), \quad k = 0, 1, \dots, 2n-1. \quad (2.1.14)$$

This system is nonlinear and is obtained from the Taylor series expansion for $f \in C^{2n}[-1, 1]$. Let us denote $I(x^k) = c_k$. We will solve the system (2.1.14) by eliminating the linear unknowns A_i . The following method illustrates it for $n = 3$ (thus, $2n - 1 = 5$), and its generalization to an arbitrary finite value of n is straightforward. First, we use the Gauss elimination method to solve the system:

$$\begin{aligned} A_1 + A_2 + A_3 &= c_0, \\ A_1 x_1 + A_2 x_2 + A_3 x_3 &= c_1, \\ \dots \\ A_1 x_1^5 + A_2 x_2^5 + A_3 x_3^5 &= c_5. \end{aligned}$$

Also, for $k = 0, 1, 2$,

$$c_k x_1 x_2 x_3 - c_{k+1} (x_1 x_2 + x_1 x_3 + x_2 x_3) + c_{k+2} (x_1 + x_2 + x_3) - c_{k+3} = 0,$$

*This is also known as *Kepler's barrel rule* since it was used to evaluate the volume of a barrel by rotating its defining contour.

This yields the Vieta coefficients

$$V_1 = x_1 + x_2 + x_3, \quad V_2 = x_1x_2 + x_1x_3 + x_2x_3, \quad V_3 = x_1x_2x_3,$$

the nodal polynomial

$$\omega_3(x) = (x - x_1)(x - x_2)(x - x_3) = x^3 - V_1x^2 + V_2x - V_3,$$

and the weights

$$\begin{aligned} A_1 &= \frac{c_0x_2x_3 - c_1(x_2 + x_3) + c_2}{(x_2 - x_1)(x_3 - x_1)}, & A_2 &= \frac{c_0x_1x_3 - c_1(x_1 + x_3) + c_2}{(x_1 - x_2)(x_3 - x_2)}, \\ A_3 &= \frac{c_0x_1x_2 - c_1(x_1 + x_2) + c_2}{(x_1 - x_3)(x_2 - x_3)}. \end{aligned} \tag{2.1.15}$$

EXAMPLE 2.1.4. This example computes the nodes and the weights of a three-point quadrature formula with $w(x) = 1$. For the integral $I_a^b(f)$ we determine the weights A_i and the nodes x_i in Q_3f . We have $c_0 = 2$, $c_2 = 2/3$, $c_4 = 2/5$, and $c_1 = c_3 = c_5 = 0$. The Vieta coefficients are $V_1 = V_3 = 0$, and $V_2 = -3/5$, thus, $\omega_3(x) = x^3 - (3/5)x$, and its zeros are $x_1 = -\sqrt{3/5}$, $x_2 = 0$, $x_3 = \sqrt{3/5}$. Hence, the weights are $A_1 = A_3 = 5/9$, $A_2 = 8/9$. ■

2.2. Euler-Maclaurin Expansion

Three important formulas are presented in this section. They are: Darboux's formula, Bernoulli numbers and Bernoulli polynomials, and the Euler-Maclaurin formula.

2.2.1. Darboux's Formula. Let $f(x)$ be analytic at all points of the interval $[a, x]$, and let $\phi(t) \in \mathcal{P}_n$. If $t \in [0, 1]$, we have by differentiation

$$\begin{aligned} \frac{d}{dt} \sum_{m=1}^n (-1)^m (x-a)^m \phi^{(n-m)}(t) f^{(m)}(a+t(x-a)) \\ = -(x-a) \phi^{(n)}(t) f'(a+t(x-a)) \\ + (-1)^n (x-a)^{n+1} \phi(t) f^{(n+1)}(a+t(x-a)). \end{aligned}$$

Since $\phi^{(n)}(t) = \phi^{(n)}(0) = \text{const}$, we integrate from 0 to 1 with respect to t and obtain

$$\begin{aligned} \phi^{(n)}(0) [f(x) - f(a)] \\ = \sum_{m=1}^n (-1)^{m-1} (x-a)^m \{ \phi^{(n-m)}(1) f^{(m)}(x) - \phi^{(n-m)}(0) f^{(m)}(0) \} \\ + (-1)^n (x-a)^{n+1} \int_0^1 \phi(t) f^{(n+1)}(a+t(x-a)) dt, \end{aligned} \tag{2.2.1}$$

which is known as *Darboux's formula*. Taylor's series is a particular case of (2.2.1) by setting $\phi(t) = (t - 1)^n$ and letting $n \rightarrow \infty$.

2.2.2. Bernoulli Numbers and Bernoulli Polynomials. The function $\frac{z}{2} \cot \frac{z}{2}$ is analytic for $|z| < 2\pi$, and being an even function of z it can be expanded into a Maclaurin series

$$\frac{z}{2} \cot \frac{z}{2} = 1 - B_1 \frac{z^2}{2!} - B_2 \frac{z^4}{4!} - B_4 \frac{z^6}{6!} - \dots, \quad (2.2.2)$$

where B_n is known as the n -th *Bernoulli number*. Some values are $B_1 = 1/6$, $B_2 = 1/30$, $B_3 = 1/42$, $B_4 = 1/30$, $B_5 = 5/66$, \dots . These numbers can be expressed as definite integrals by

$$B_n = 4n \int_0^\infty \frac{t^{2n-1}}{e^{2\pi t} - 1} dt. \quad (2.2.3)$$

The Bernoulli polynomials $B_n(x)$ of order n are defined as the coefficients of $\frac{t^n}{n!}$ in the Maclaurin expansion of the function $t \frac{e^{xt} - 1}{e^t - 1}$, so that

$$t \frac{e^{xt} - 1}{e^t - 1} = \sum_{n=1}^{\infty} \frac{B_n(x) t^n}{n!}. \quad (2.2.4)$$

Some properties of this polynomial are:

1. Set $x + 1$ in place of x in (2.2.4) and subtract; this gives

$$t e^{xt} = \sum_{n=1}^{\infty} \{B_n(x+1) - B_n(x)\} \frac{t^n}{n!}.$$

By equating the coefficients of t^n on both sides of this equation, we obtain

$$n x^{n-1} = B_n(x+1) - B_n(x), \quad (2.2.5)$$

which is a difference equation satisfied by $B_n(x)$.

2. An explicit expression for the Bernoulli polynomials is

$$B_n(x) = x^n - \frac{1}{2} n x^{n-1} + \binom{n}{2} B_1 x^{n-2} - \binom{n}{4} B_2 x^{n-4} + \binom{n}{6} B_3 x^{n-6} - \dots, \quad (2.2.6)$$

the last term of which is in x or x^2 . In particular, if x is an integer, then we find from (2.2.5) that $\frac{B_n(x)}{n} = 1^{n-1} + 2^{n-1} + \dots + (x-1)^{n-1}$.

2.2.3. Euler-Maclaurin Expansion Formula. If we write $B_n(t)$ for $\phi(t)$ in Darboux's formula (2.2.1), and differentiate $(n-k)$ times the equation (2.2.5), where x is replaced by t , then we get

$$B_n^{(n-k)}(t+1) - B_n^{(n-k)}(t) = n(n-1) \dots k t^{k-1}.$$

Set $t = 0$ in this equation, which gives $B_n^{(n-k)}(1) = B_n^{(n-k)}(0)$. Now, from the Maclaurin series for $B_n(x)$, we have for $k > 0$

$$\begin{aligned} B_n^{(n-2k-1)}(0) &= 0, & B_n^{(n-2k)}(0) &= (-1)^{k-1} \frac{n!}{(2k)!} B_k, \\ B_n^{(n-1)}(0) &= -\frac{1}{2} n!, & B_n^{(n)}(0) &= n!. \end{aligned}$$

Substituting these values of $B_n^{(n-k)}(1)$ and $B_n^{(n-k)}(0)$ into (2.2.1), we obtain the *Euler-Maclaurin sum formula*

$$\begin{aligned} (x-a)f'(a) &= f(x) - f(a) - \frac{x-a}{2} \{f'(x) - f'(a)\} \\ &+ \sum_{m=1}^{n-1} \frac{(-1)^{m-1} B_m (x-a)^{2m}}{(2m)!} \{f^{(2m)}(x) - f^{(2m)}(a)\} \\ &- \frac{(x-a)^{2n+1}}{(2n)!} \int_0^1 B_{2n}(t) f^{(2n+1)}(a+t(x-a)) dt. \end{aligned} \quad (2.2.7)$$

In certain cases the last term tends to zero as $n \rightarrow \infty$, which gives an infinite series for $f(x) - f(a)$. If we set h for $x-a$ and $F(x)$ for $f'(x)$ in formula (2.2.7), we get

$$\begin{aligned} \int_a^{a+h} F(x) dx &= \frac{h}{2} \{F(a) + F(a+h)\} \\ &+ \sum_{m=1}^{n-1} \frac{(-1)^m B_m h^{2m}}{(2m)!} \{F^{(2m-1)}(a+h) - f^{(2m-1)}(a)\} \\ &- \frac{h^{2n+1}}{(2n)!} \int_0^1 B_{2n}(t) F^{(2n)}(a+th) dt. \end{aligned}$$

Then writing $a+h, a+2h, \dots, a+(r-1)h$ for a in this result and adding all of them, we obtain

$$\begin{aligned} \int_a^{a+rh} F(x) dx &= h \sum_{k=0}^r F(a+kh) \\ &+ \sum_{m=1}^{n-1} \frac{(-1)^m B_m h^{2m}}{(2m)!} \{F^{(2m-1)}(a+rh) - f^{(2m-1)}(a)\} + R_n, \end{aligned} \quad (2.2.8)$$

where

$$R_n = \frac{h^{2n+1}}{(2n)!} \int_0^1 B_{2n}(t) \left\{ \sum_{m=0}^{r-1} F^{(2n)}(a+mh+th) \right\} dt.$$

Formula (2.2.8) is very useful in numerically evaluating definite integrals. It is valid if $F(x)$ is analytic at all points of the interval $[a, a + rh]$.

2.3. Interpolatory Quadrature Rules

Interpolatory polynomials are used to develop quadrature formulas for integrating a function $f(x)$ over the interval $[a, b]$. We choose n points (nodes or abscissae) x_k , $k = 1, 2, \dots, n$, in this interval. If the function $f(x)$ is defined over the interval $[a, b]$, then we must choose these n points x_k , $k = 1, 2, \dots, n$, entirely in the interval $[a, b]$. But if $f(x)$ is defined outside the interval of integration, then all x_k need not belong to $[a, b]$. Quadrature formulas which contain some nodes lying outside $[a, b]$ are discussed in Garloff et al. (1986). However, for integration of real integrable functions all the nodes x_k must belong to the interval of integration.

2.3.1. General Integration Rules. Let the interpolating polynomial $p(x)$ for $f(x)$ be such that

$$f(x) = p(x) + r(x), \quad (2.3.1)$$

where $r(x)$ is the remainder of the integration, and

$$p(x) = \sum_{k=1}^n \frac{\pi(x)}{(x - x_k) \pi'(x_k)} f(x_k),$$

$$\pi(x) = (x - x_1)(x - x_2) \dots (x - x_n). \quad (2.3.2)$$

Then the exact value of the integral of the product $w(x)f(x)$ over the interval $[a, b]$ is

$$\int_a^b w(x)f(x) dx = \int_a^b w(x)p(x) dx + \int_a^b w(x)r(x) dx. \quad (2.3.3)$$

The behavior of the remainder $r(x)$ depends on the preciseness of the interpolating polynomial $p(x)$. Thus, if $r(x)$ is small throughout the interval $[a, b]$, then the second term in Eq (2.3.3) can be neglected. This situation leads to the approximate equation

$$\int_a^b w(x)f(x) dx \approx \sum_{k=1}^n A_k f(x_k), \quad (2.3.4)$$

where

$$A_k = \int_a^b w(x) \frac{\pi(x)}{(x - x_k) \pi'(x_k)} dx. \quad (2.3.5)$$

Formulas of the type (2.3.4) are called *interpolatory quadrature formulas*. The necessary and sufficient condition for the quadrature formula (2.3.4) to be interpolatory is that it be exact for all possible polynomials $p(x)$ of degree at most $n - 1$.

For a proof of formula (2.3.4) see Krylov 1962, p. 80. Once all n nodes x_k are specified, formula (2.3.4) is completely defined, because then the coefficients A_k are completely evaluated.

The remainder $R(f)$ of the rule (2.3.4) is defined by

$$R(f) \equiv \int_a^b w(x) f(x) dx = \int_a^b w(x) \pi(x) f(x, x_1, \dots, x_k) dx. \quad (2.3.6)$$

If $f \in C^n[a, b]$, then $R(f)$ can be represented in the form

$$R(f) = \int_a^b \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} w(x) \pi(x) f^{(n)}\left(x + \sum_{k=0}^n t_k (x_k - x_{k-1})\right) dt_n \cdots dt_1 dx, \quad (2.3.7)$$

where $x = x_0$ (see Krylov 1962, p. 81). But if we use the Lagrangian form of $r(x)$, which is

$$r(x) = \frac{1}{n!} \pi(x) f^{(n)}(\xi), \quad a < \xi < b,$$

then

$$R(f) = \frac{1}{n!} \int_a^b w(x) \pi(x) f^{(n)}(\xi) dx. \quad (2.3.8)$$

This expression for $R(f)$ does not yield an exact bound for $R(f)$ because we cannot determine how ξ depends on x . But if $|f^{(n)}(x)| \leq M_n$ for all $x \in [a, b]$, then from (2.3.8) we get

$$|R(f)| \leq \frac{M_n}{n!} \int_a^b |w(x) \pi(x)| dx. \quad (2.3.9)$$

If the product $w(x) \pi(x)$ does not change sign on the interval $[a, b]$, then the bound (2.3.9) cannot be improved. However, for arbitrary $w(x)$ and an arbitrary sequence of n nodes x_k we have

$$R(f) = \int_a^b K(t) f^{(n)}(t) dt, \quad (2.3.10)$$

where the kernel $K(t)$ is defined by

$$K(t) = \int_a^b w(x) [U(x-t) - U(a-t)] \frac{(x-t)^{n-1}}{(n-1)!} dx - \sum_{k=1}^n A_k [U(x_k-t) - U(a-t)] \frac{(x_k-t)^{n-1}}{(n-1)!}, \quad (2.3.11)$$

and if $t \neq a$ and $t \neq x_k, k = 1, \dots, n$, then

$$K(t) = \begin{cases} -\int_a^t w(x) \frac{(x-t)^{n-1}}{(n-1)!} dx + \sum_{x_k < t} A_k \frac{(x-t)^{n-1}}{(n-1)!} & \text{if } t < a, \\ \int_a^t w(x) \frac{(x-t)^{n-1}}{(n-1)!} dx - \sum_{x_k > t} A_k \frac{(x-t)^{n-1}}{(n-1)!} & \text{if } t > a. \end{cases} \quad (2.3.12)$$

Finally, if $|f^{(n)}(x)| \leq M_n$ for $x \in [a, b]$, then

$$|R(f)| \leq M_n \int_a^b |K(t)| dt. \quad (2.3.13)$$

2.3.2. Lagrange Formula. This formula for the interval $[a, b]$ is

$$I_a^b(f) = \sum_{k=0}^n \left(L_k^{(n)}(b) - L_k^{(n)}(a) \right) f_k + R_n, \quad (2.3.14)$$

where

$$\begin{aligned} L_k^{(n)}(x) &= \frac{1}{\pi'_n(x_k)} \int_{x_0}^x \frac{\pi(t)}{t - x_k} dt = \int_{x_0}^x l_k(t) dt, \\ l_k(x) &= \frac{\pi_n(x)}{(x - x_k) \pi'_n(x)} = \frac{(x - x_0) \dots (x - x_{k-1})(x - x_{k+1}) \dots (x - x_n)}{(x_k - x_0) \dots (x_k - x_{k-1})(x_k - x_{k+1}) \dots (x_k - x_n)}, \\ R_n &= \frac{1}{(n+1)!} \int_a^b \pi_n(x) f^{(n+1)}(\xi(x)) dx, \end{aligned}$$

For an equally-spaced quadrature points x_k this formula becomes

$$\int_{x_0}^{x_n} f(x) dx = \frac{1}{h^n} \sum_{i=0}^n f_i \frac{(-1)^{n-i}}{i!(n-i)!} \int_{x_0}^{x_k} \frac{\pi_n(x)}{x - x_i} dx + R_n, \quad (2.3.15)$$

$$\int_{x_0}^{x_{m+1}} f(x) dx = h \sum_{i=-\lfloor (n-1)/2 \rfloor}^{\lfloor n/2 \rfloor} A_i(m) f_i + R_n, \quad (2.3.16)$$

where $A_i(m)$ denote the Lagrangian integration coefficients available in Abramowitz and Stegun (1968, p. 915).

2.4. Newton-Cotes Formulas

Consider the definite integral $I_a^b(f) = \int_a^b f(x) dx$. We partition the interval $[a, b]$ into n equal subintervals of length $h = (b - a)/n$ at the points $a, a + h, a + 2h, \dots, a +$

$nh = b$. We will derive interpolatory quadrature formulas using these points as nodes. The values of the coefficients A_k in formula (2.3.4) are determined in a form that is independent of the interval $[a, b]$. Thus, we write (2.3.4) as

$$\int_a^b f(x) dx = (b-a) \sum_{k=0}^n C_k^n f(a+kh), \quad (2.4.1)$$

which is known as the *Newton-Cotes formula*, where the coefficients C_k^n are given by

$$C_k^n = A_k/(b-a) = \frac{1}{b-a} \int_a^b \frac{\pi(x)}{(x-a-kh)\pi'(a+kh)} dx, \quad (2.4.2)$$

$$\pi(x) = (x-a)(x-a-h)(x-a-2h)\dots(x-a-nh).$$

If we set $x = a + th$, then

$$\begin{aligned} x-a-kh &= h(t-k), \\ \pi(x) &= h^{n+1}t(t-1)(t-2)\dots(t-n), \\ \pi'(a+kh) &= (-1)^{n-k}h^n k!(n-k)!. \end{aligned}$$

Then

$$C_k^n = \frac{(-1)^{n-k}}{n k!(n-k)!} \int_0^n t(t-1)(t-2)\dots(t-k+1)(t-k-1)\dots(t-n) dt. \quad (2.4.3)$$

The coefficients C_k^n are known as the *Cotesian numbers*. Some of these numbers are tabulated in [Table A.1](#) for $k \leq n/2$, since $C_k^n = C_{n-k}^n$. A table of Cotesian numbers for $n = 1(1)20$ is available as the file [CotesianNumbers.pdf](#) on the CD-R; also, see [Kopal](#) (1961) and [Johnson](#) (1915) where a short history of the Cotesian numbers is also given.

In order to understand the behavior of the Newton-Cotes formula (2.4.1) for a large number of nodes, we will derive the asymptotic representation for C_k^n for large n . First, we write the integral in (2.1.8) as

$$I = \int_0^n \frac{x(x-1)\dots(x-n)}{x-k} dx. \quad (2.4.4)$$

Since $x(x-1)\dots(x-n) = \frac{\Gamma(x+1)}{\Gamma(x-n)}$, and $\frac{1}{\Gamma(x)} = \frac{\Gamma(1-x) \sin \pi x}{\pi}$, we get

$$x(x-1)\dots(x-n) = \frac{(-1)^n}{\pi} \Gamma(x+1)\Gamma(n+1-x) \sin \pi x,$$

and thus,

$$\begin{aligned}
 I &= (-1)^n \int_0^n \frac{\Gamma(x+1)\Gamma(n+1-x) \sin \pi x}{\pi(x-k)} dx \\
 &= (-1)^n \left(\int_0^3 + \int_3^{n-3} + \int_{n-3}^n \right) \frac{\Gamma(x+1)\Gamma(n+1-x) \sin \pi x}{\pi(x-k)} dx \\
 &\equiv I_1 + I_2 + I_3,
 \end{aligned} \tag{2.4.5}$$

Now, since $\frac{\Gamma'(z)}{\Gamma(z)} = -\frac{1}{z} - C + \sum_{k=1}^{\infty} \left(\frac{1}{k} - \frac{1}{k+z} \right)$ is a monotone increasing function for $z > 0$, we notice that by using Taylor's formula the derivative of the function $\frac{\Gamma'(z)}{\Gamma(z)}$ is of the order $1/z$ for large z . Thus,

$$\ln \Gamma(n+1-x) = \ln \Gamma(n+1) - \frac{x\Gamma'(n+1)}{\Gamma(n+1)} + O\left(\frac{1}{n}\right).$$

Then since for large z using the approximation $\frac{\Gamma'(z)}{\Gamma(z)} = \ln z + O\left(\frac{1}{z}\right)$, we find that

$$\Gamma(n+1-x) = \Gamma(n+1) e^{-x \ln n} \left[1 + O\left(\frac{1}{n}\right) \right]. \text{ Also, for } 0 \leq x \leq 3,$$

$$\Gamma(x+1) \frac{\sin \pi x}{\pi(x-k)} = -\frac{x}{k} + O\left(\frac{x^2}{k}\right),$$

and

$$\begin{aligned}
 \int_0^3 x e^{-x \ln n} dx &= \frac{1}{\ln^2 n} - \frac{1}{n^3} \left[\frac{3}{\ln n} + \frac{1}{\ln^2 n} \right], \\
 \int_0^3 x^2 e^{-x \ln n} dx &= \frac{2}{\ln^3 n} - \frac{1}{n^3} \left[\frac{9}{\ln n} + \frac{6}{\ln^2 n} + \frac{2}{\ln^3 n} \right],
 \end{aligned}$$

which gives

$$\begin{aligned}
 I_1 &= \int_0^3 \Gamma(n+1) e^{-x \ln n} \left[1 + O\left(\frac{1}{n}\right) \right] \left[-\frac{x}{k} + O\left(\frac{x^2}{k}\right) \right] dx \\
 &= -\frac{\Gamma(n+1)}{k \ln^2 n} \left[1 + O\left(\frac{1}{\ln n}\right) \right] \quad \text{for } 1 \leq k \leq n-1.
 \end{aligned} \tag{2.4.6}$$

Similarly,

$$I_3 = (-1)^{n-1} \frac{\Gamma(n+1)}{(n-k) \ln^2 n} \left[1 + O\left(\frac{1}{\ln n}\right) \right] \quad \text{for } 1 \leq k \leq n-1. \tag{2.4.7}$$

Now, for the integral I_2 note that

$$\frac{\Gamma'(x+2)}{\Gamma(x+1)} - \frac{\Gamma'(n+1-x)}{\Gamma(n+1-x)} \begin{cases} < 0 & \text{for } -1 < x < n/2, \\ > 0 & \text{for } n/2 < x < n+1. \end{cases}$$

This implies that for $3 \leq x \leq n-3$ the quantities $\ln \Gamma(x+1)\Gamma(n+1-x)$ and $\Gamma(x+1)\Gamma(n+1-x)$ will have their largest value at the endpoints of this interval, i.e.,

$$0 < \Gamma(x+1)\Gamma(n+1-x) \leq \Gamma(4)\Gamma(n-2) = 6\Gamma(n-2).$$

Since $\left| \frac{\sin \pi x}{\pi(x-k)} \right| \leq 1$, we have

$$|I_2| \leq 6n\Gamma(n-2) = \frac{6\Gamma(n+1)}{(n-2)(n-1)} = O\left(\frac{\Gamma(n+1)}{n_2}\right). \quad (2.4.8)$$

Thus, combining (2.4.6), (2.4.7), and (2.4.8), we find that

$$I = \frac{(-1)^{n-1}\Gamma(n+1)}{\ln^2 n} \left[\frac{1}{k} + \frac{(-1)^n}{n-k} \right] \left[1 + O\left(\frac{1}{\ln n}\right) \right]. \quad (2.4.9)$$

This yields the following asymptotic representation for the Cotesian numbers for $1 \leq k \leq n-1$:

$$B_k^n = \frac{(-1)^{k-1}n!}{k!(n-k)!n\ln^2 n} \left[\frac{1}{k} + \frac{(-1)^n}{n-k} \right] \left[1 + O\left(\frac{1}{\ln n}\right) \right]. \quad (2.4.10)$$

Note that

$$C_0^n = C_n^n = \frac{1}{n\ln n} \left[1 + O\left(\frac{1}{\ln n}\right) \right]. \quad (2.4.11)$$

From the expressions (2.4.10) and (2.4.11) it is obvious that the Newton-Cotes formulas will have both positive and negative coefficients which in absolute value exceed any arbitrary large number. Thus, for large n , a small discrepancy in the values of the function $f(a+kh)$ can generate a larger error in the quadrature sum. It is for this reason that the Newton-Cotes formulas with larger number of nodes are not very useful in practice. Now, we consider the following two cases.

CASE 1. When n is an even number, the Newton-Cotes formulas will have an odd number of nodes. In this case the function $\pi(x)$ is such that $\pi(a+z) = -\pi(a+n h-z)$, where $z < b-a$, and the graph of $\pi(x)$ will be symmetric with respect to the midpoint $(a+b)/2$ of the interval $[a, b]$. If $f \in C^{n+2}[a, b]$, then the remainder $R(f)$ can be expressed as

$$R(f) = \frac{f^{(n+2)}(\xi)}{(n+2)!} \int_a^b x \pi(x) dx, \quad a < \xi < b, \quad (2.4.12)$$

and the coefficient of $f^{(n+2)}(\xi)$ is negative. This result implies that if the number of nodes in formula (2.4.1) is odd, then the algebraic degree of precision in this formula is $n + 1$. Thus, from (2.4.12) which represents error, formula (2.4.1) will be exact whenever $f(x)$ is a polynomial of degree $\leq n + 1$. If $f(x)$ is a polynomial of degree $n + 2$, then $f^{(n+2)}(x)$ will be nonzero and $R(f) \neq 0$. The error $R(f)$ can also be expressed in terms of the kernel $K(t)$ as

$$R(f) = \int_a^b f^{(n+2)}(t) K(t) dt, \quad (2.4.13)$$

where $K(t) \leq 0$ on $[a, b]$ and is given by

$$K(t) = \frac{(b-t)^{n+2}}{(n+2)!} - \sum_{k=1}^n A_k U(a+kh-t) \frac{(a+kh-t)^{n+1}}{(n+1)!}. \quad (2.4.14)$$

CASE 2. When n is an odd number, there are an even number of nodes in formula (2.4.1). The polynomial $\pi(x)$ takes the same value at both the points $a+t$ and $b-t$, where $t < b-a$. It means that the graph of $\pi(x)$ will be symmetric with respect to the line $x = (a+b)/2$. If $f \in C^{n+1}[a, b]$, then the remainder $R(f)$ can be expressed as

$$R(f) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_a^b \pi(x) dx, \quad a < \xi < b, \quad (2.4.15)$$

and the coefficient of $f^{(n+1)}(\xi)$ is negative. As in the above case, this result implies that if the Newton-Cotes formula (2.4.1) has an even number of nodes, then its algebraic degree of precision is $n + 1$. The error $R(f)$ can also be expressed in terms of the kernel $K(t)$ as

$$R(f) = \int_a^b f^{(n+1)}(t) K(t) dt, \quad (2.4.16)$$

where $K(t) \leq 0$ on $[a, b]$ and is given by

$$K(t) = \frac{(b-t)^{n+1}}{(n+1)!} - \sum_{k=1}^n A_k U(a+kh-t) \frac{(a+kh-t)^n}{n!}. \quad (2.4.17)$$

2.4.1. Closed-Type Newton-Cotes Rules. We write the rule (2.4.1) as

$$I_a^b(f) = (b-a) \sum_{k=0}^n w_k f(x_k),$$

where $\sum_{k=0}^n w_k = 1$. The weights w_k for $n = 1, 2, \dots, 11$ are given in [Table A.1](#). For $n = 1$ this formula gives the basic rectangle rule; for $n = 2$ it gives Simpson's two-strip rule, and for $n = 3, \dots, 10$ it gives the following rules:

1. SIMPSON'S 3/8 RULE.

$$\int_{x_0}^{x_3} f(x) dx = \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(\xi).$$

2. BODE'S (FOUR-STRIP) RULE.

$$\int_{x_0}^{x_4} f(x) dx = \frac{2h}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945} f^{(6)}(\xi).$$

3. FIVE-STRIP RULE.

$$\int_{x_0}^{x_5} f(x) dx = \frac{5h}{288} (19f_0 + 75f_1 + 50f_2 + 50f_3 + 75f_4 + 19f_5) - \frac{275h^7}{12096} f^{(6)}(\xi).$$

4. SIX-STRIP RULE.

$$\int_{x_0}^{x_6} f(x) dx = \frac{h}{140} (41f_0 + 216f_1 + 27f_2 + 272f_3 + 27f_4 + 216f_5 + 41f_6) - \frac{9h^9}{1400} f^{(8)}(\xi).$$

5. SEVEN-STRIP RULE.

$$\int_{x_0}^{x_7} f(x) dx = \frac{7h}{17280} (751f_0 + 3577f_1 + 1323f_2 + 2989f_3 + 2989f_4 + 1323f_5 + 3577f_6 + 751f_7) - \frac{8183h^9}{518400} f^{(8)}(\xi).$$

6. EIGHT-STRIP RULE.

$$\int_{x_0}^{x_8} f(x) dx = \frac{4h}{14175} (989f_0 + 5888f_1 - 928f_2 + 10496f_3 - 4540f_4 + 10496f_5 - 928f_6 + 5888f_7 + 989f_8) - \frac{2368h^{11}}{467775} f^{(10)}(\xi).$$

7. NINE-STRIP RULE.

$$\int_{x_0}^{x_9} f(x) dx = \frac{9h}{89600} [2857(f_0 + f_9) + 15741(f_1 + f_8) + 1080(f_2 + f_7) + 19344(f_3 + f_6) + 5778(f_4 + f_5)] - \frac{173h^{11}}{14620} f^{(10)}(\xi).$$

8. TEN-STRIP RULE.

$$\int_{x_0}^{x_{10}} f(x) dx = \frac{5h}{299376} [16067 (f_0 + f_{10}) + 106300 (f_1 + f_9) \\ - 48525 (f_2 + f_8) + 272400 (f_3 + f_7) - 260550 (f_4 + f_6) \\ + 427368 f_5] - \frac{1346350 h^{13} f^{(12)}(\xi)}{326918592}.$$

A simple guideline to use the Newton-Cotes rule is as follows: When n is even (i.e., when there is an even number of subintervals or an odd number of base points), this rule is exact when $f(x)$ is a polynomial of degree $n + 1$ or less; when n is odd, this rule is exact for polynomials of degree n or less; conversely, a polynomial of degree n is integrated exactly by choosing $n + 1$ base points.

Smith (1965) gives two compound N-C rules on the interval $[-1, 1]$, which are

1. 7-8 RULE:

$$\int_{-1}^1 f(x) dx = \frac{\pi}{15n} \left[7 \sum_{k=1}^{n-1} g(k\pi/n) + 8 \sum_{k=1}^n g(k-1/2)\pi/n \right] \\ + \frac{\pi^2}{60n^2} [f(-1) + f(1)] + O(n^{-6});$$

2. 31-32 RULE:

$$\int_{-1}^1 f(x) dx = \frac{\pi}{63n} \left[31 \sum_{k=1}^{n-1} g(k\pi/n) + 32 \sum_{k=1}^n g(k-1/2)\pi/n \right] \\ + \left[\frac{5}{63} + \frac{1}{945} \left(\frac{\pi}{2n} \right)^2 \right] \left(\frac{\pi}{2n} \right)^2 [f(-1) + f(1)] \\ + \frac{1}{315} \left(\frac{\pi}{2n} \right)^4 [f'(1) - f'(-1)] + O(n^{-8}),$$

where $g(x) = \sin x f(\cos x)$. These rules are somewhat similar to the Clenshaw-Curtis rules (see §4.3.4).

The *non-repeated* trapezoidal and Simpson's rules are special cases of the closed Newton-Cotes formulas (2.4.1), which can be written as

$$\int_{x_0}^{x_n} f(x) dx \approx \sum_{i=0}^n w_i f(x_0 + ih). \quad (2.4.18)$$

For example, for $n = 3$ we have the weights $w_0 = w_3 = 3h/8$, $w_1 = w_2 = 9h/8$. For even n these formulas are exact if f is a polynomial of degree $n + 1$. Note this for the Simpson's rule for $n = 2$ given above.

2.4.2. Open-Type Newton-Cotes Rules. These formulas have the form

$$\int_{x_0}^{x_n} f(x) dx \approx \sum_{i=0}^{n-1} w_i f(x_0 + ih). \quad (2.4.19)$$

The terms ‘closed’ and ‘open’ refer to whether the endpoints x_0 and x_n are included or not included in the formula. Using (2.4.19) the simplest N-C rule over the interval $[x_0 - h, x_0 + h]$ is

$$\begin{aligned}\int_{x_0-h}^{x_0+h} f(x) dx &= 2h f_0 + h^3 \int_{-1}^1 \binom{s}{2} f''(\xi_x) ds \\ &= 2h f_0 + \frac{1}{3} h^3 f''(\xi_x).\end{aligned}$$

If we apply this rule over the interval $[x_0, x_1]$, we get

$$\int_{x_0}^{x_1} f(x) dx = h f\left(x_0 + \frac{h}{2}\right) + \frac{h^3}{24} f''(\xi), \quad x_0 < \xi < x_1, \quad (2.4.20)$$

which is known as the *midpoint rule*. The repeated midpoint rule is

$$\int_{x_0}^{x_N} f(x) dx = h \sum_{j=0}^{N-1} f\left(x_j + \frac{h}{2}\right) + (x_N - x_0) \frac{h^2}{24} f''(\xi), \quad x_0 < \xi < x_N, \quad (2.4.21)$$

Some specific formulas are as follows:

1. $\int_{x_0}^{x_3} f(x) dx = \frac{3h}{2} (f_1 + f_2) + \frac{h^3}{4} f''(\xi).$
2. $\int_{x_0}^{x_4} f(x) dx = \frac{4h}{3} (2f_1 - f_2 + 2f_3) + \frac{28h^5}{90} f^{(4)}(\xi).$
3. $\int_{x_0}^{x_5} f(x) dx = \frac{5h}{24} (11f_1 + f_2 + f_3 + 11f_4) + \frac{95h^5}{144} f^{(4)}(\xi).$
4. $\int_{x_0}^{x_6} f(x) dx = \frac{6h}{20} (11f_1 - 14f_2 + 26f_3 - 14f_4 + 11f_5) + \frac{41h^7}{140} f^{(6)}(\xi).$
5. $\int_{x_0}^{x_7} f(x) dx = \frac{7h}{1440} (611f_1 - 463f_2 + 562f_3 + 562f_4 - 453f_5 + 611f_6) \\ + \frac{5257h^7}{8640} f^{(6)}(\xi).$
6. $\int_{x_0}^{x_8} f(x) dx = \frac{8h}{945} (460f_1 - 954f_2 + 2196f_3 - 2459f_4 + 2196f_5 \\ - 954f_6 + 460f_7) + \frac{3956h^9}{14175} f^{(8)}(\xi).$

We can obtain some integration formulas of the open type by using only the interior nodes either by making a Lagrangian fit at these interior points or by the method of undetermined coefficients used in §2.3.1 without using the terms $f(a)$ and

$f(b)$. These rules have equally spaced nodes of step size h :

$$\begin{aligned}\int_0^{3h} f(x) \, dx &= \frac{3h}{2} (f_1 + f_2) + \frac{3h^3}{4} f''(\xi), \\ \int_0^{4h} f(x) \, dx &= \frac{4h}{3} (2f_1 - f_2 + 2f_3) + \frac{14h^5}{45} f^{(4)}(\xi), \\ \int_0^{5h} f(x) \, dx &= \frac{5h}{24} (11f_1 + f_2 + f_3 + 11f_4) + \frac{95h^5}{144} f^{(4)}(\xi), \\ \int_0^{6h} f(x) \, dx &= \frac{3h}{10} (11f_1 - 14f_2 + 2f_3 - 14f_4 + 11f_5) + \frac{41h^7}{140} f^{(6)}(\xi),\end{aligned}$$

where $f_i = f(ih)$, and ξ is an interior point of the interval of integration. Since these rules have alternately plus and minus signs, they will show instabilities, but they are useful for integrals with endpoint singularities, thus enabling the computation of singular integrals which are discussed in detail in [Chapter 5](#).

Note that the midpoint rule (2.4.20) requires only one evaluation of f , as compared to two in the trapezoidal rule, although (2.4.20) has high accuracy of order h^3 . Also the repeated midpoint rule (2.4.21) requires N evaluations of f , which are only one less than those required by the repeated trapezoidal rule. It would appear that the midpoint rule (2.4.20) is better than the trapezoidal rule, but this observation is misleading. In fact, if f'' has the same sign in $[x_0, x_N]$, the exact value of the integral lies between the values computed by the midpoint and the trapezoidal rules. The following examples illustrate this remark.

EXAMPLE 2.4.1. Compute $\int_0^1 \frac{dx}{1+x}$. The results are given in Table 2.4.1. The exact value is 0.69314718.

Table 2.4.1.

n	Trapezoidal	Midpoint	Simpson's
1	0.750000	0.666667	—
2	0.708333	0.685714	0.694444
3	0.7000	0.689755	—
4	0.697024	0.691219	0.693254
5	0.695635	0.691908	—
6	0.694877	0.692284	0.693149

EXAMPLE 2.4.2. Compute $\int_0^1 \frac{dx}{1+x^2}$. The results are given in [Table 2.4.2](#).

The exact value is $\tan^{-1}(1) \approx 0.785398$.

Table 2.4.2.

n	Trapezoidal	Midpoint	Simpson's
1	0.750000	0.800000	—
2	0.775000	0.790588	0.783333
3	0.780769	0.787712	—
4	0.782794	0.786700	0.785392
5	0.783732	0.786231	—
6	0.784241	0.785977	0.785398

Note that (i) Newton-Cotes rules are Riemann sums; thus, if $n \rightarrow \infty$, they converge to the exact value of the integral; and (ii) Trapezoidal rule T_n is sometimes modified to Romberg's scheme (see §3.5) or Gregory's scheme (see §3.6). These schemes provide modifications of this rule with an end correction.

If we rewrite the formula (2.4.1) in the form

$$I_a^b(f) = \int_0^{mj} f(x) dx \approx \sum_{j=0}^m w_{jm} f(jh), \quad m = 1, 2, \dots, n, \quad (2.4.22)$$

then the weights w_{mj} for some useful quadrature rules are given in [Tables A.2, A.3, A.4](#) and [A.5](#) (Baker 1978, p. 120).

2.5. Basic Quadrature Rules

A classical quadrature rule has the form

$$I_a^b(wf) \equiv \int_a^b w(x) f(x) dx = \sum_{k=1}^n w_k f(x_k) + E_n,$$

where $w(x)$ denotes a weight function, w_k are the weights, x_k the nodes or abscissae (or quadrature points), $n \in \mathbb{Z}^+$, and E_n the error term. The first basic rule is obtained from the left-hand Riemann sum

$$I_a^b(f) \approx h \sum_{k=0}^{n-1} f(a + kh) = R_n^{(1)}(f), \quad h = \frac{b-a}{n},$$

and the right-hand Riemann sum

$$I_a^b(f) \approx h \sum_{k=1}^n f(a + kh) = R_n^{(2)}(f).$$

These are known as the *rectangular rules*. The second basic rule is the *midpoint rule*

$$I_a^b(f) \approx h \sum_{k=0}^{n-1} f\left(a + \left(k + \frac{1}{2}\right)h\right) = M_n(f),$$

and the third basic rule is the average of the two rectangular rules

$$I_a^b(f) \approx h \sum_{k=1}^n [f(a) + 2f(a + (k-1)h) + f(b)] = T_n(f),$$

which is the well-known *trapezoidal rule*. The rules $M_n(f)$ and $T_n(f)$ are exact for linear function $f(x)$.

The procedure to construct new quadrature rules from the basic rules is simple and it is achieved first by fitting the integrand $f(x)$ to a polynomial and then integrating this fit analytically to generate a new rule, although care must be taken to avoid unwanted circumlocation. For example, if $f(x)$ is fitted by a straight line through the endpoints $(a, f(a))$ and $(b, f(b))$, we obtain the basic trapezoidal rule

$$I_a^b(f) \approx \int_a^b (mx + q) dx = \frac{b-a}{2} [f(a) + f(b)],$$

where $m = \frac{f(b) - f(a)}{b-a}$ and $q = \frac{bf(a) - af(b)}{b-a}$. Thus, the trapezoidal rule is two-point and has degree 1. Similarly, the basic Simpson's rule is obtained by fitting $f(x)$ to a quadratic at the three points $(a, f(a))$, $(c, f(c))$ and $(b, f(b))$, where $c = (a+b)/2$:

$$\begin{aligned} I_a^b(f) &\approx \int_a^b (mx^2 + qx + r) dx = \frac{b-a}{2} [f(a) + 4f(c) + f(b)] \\ &= \frac{h}{3} [f(a) + 4f(c) + f(b)], \end{aligned}$$

where h is the step size (distance between the abscissae), and

$$\begin{aligned} m &= \frac{(c-b)f(a) + (a-c)f(b) + (b-a)f(c)}{(c-a)(b-c)(a-b)}, \\ q &= \frac{(b^2 - c^2)f(a) + (c^2 - a^2)f(b) + (a^2 - b^2)f(c)}{(c-a)(b-c)(a-b)}, \\ r &= \frac{bc(c-b)f(a) + ac(a-c)f(b) + ab(a-b)f(c)}{(c-a)(b-c)(a-b)}. \end{aligned}$$

The basic Simpson's rule is three-point and has degree 3, although we started with fitting f by a quadratic. This feature makes Simpson's rule more accurate and widely used. By dividing $[a, b]$ into n subintervals and applying the two-point trapezoidal rule

in each subinterval, we obtain the repeated (or extended) trapezoidal rule. Similarly, we obtain the compound Simpson's rule.

Some quadrature rules use f and its derivatives, such as in Hammer and Wicke (1960) and Patterson (1969) rules. These rules are also used widely and provide better accuracy in certain cases; the only requirement is that the derivatives of f must exist.

Another derivation of rules is based on the use of the complete set of monomials $\{1, x, \dots, x^n\}$ for $f(x)$ for some n , which generate sufficient equations to evaluate and fix the sets w_k and x_k . Certain other conditions may be imposed on these constants, such as the nodes $\{x_k\}$ are equally spaced. This approach yields a general class of formulas which are known as Newton-Cotes (N-C) rules where the nodes are equally spaced. The trapezoidal and Simpson's rules, among others, are special cases of the N-C rules.

EXAMPLE 2.5.1. Using the test functions $f_1(x) = e^{-x}$, $f_2(x) = \cos x$, $f_3(x) = \sqrt{x}$, $f_4(x) = \frac{1}{1+x^2}$, $f_5(x) = \frac{1}{1+e^x}$, $f_6(x) = X^{1/4}$, $f_7(x) = x^{1/6}$, $f_8(x) = \frac{1}{1+x^4}$, $f_9(x) = \frac{2}{2+\sin 10\pi x}$, with $[a, b] = [0, 1]$ and $h = 1/50$, the basic rules yield the results presented in Table 2.5.1. For computational details, see [ex2.5.1.nb](#) on the CD-R. ■

Table 2.5.1.

f	$R_n^{(1)}$	$R_n^{(2)}$	M_n	T_n	Simpson's	Exact
f_1	0.63846	0.62582	0.6321102	0.6321416	0.632120558	0.632120558
f_2	0.84604	0.83684	0.8414850	0.8414429	0.841470984	0.841470984
f_3	0.65609	0.67609	0.6668305	0.6660953	0.666585482	0.666666667
f_4	0.79038	0.78038	0.7854064	0.7853814	0.785398163	0.785398163
f_5	0.38219	0.37757	0.3798846	0.3798872	0.379885493	0.379885493
f_6	0.78759	0.80759	0.8003793	0.7975981	0.799452252	0.800000004
f_7	0.84328	0.86328	0.8575615	0.8575615	0.856136138	0.857142857
f_8	0.87193	0.86193	0.8669896	0.8669396	0.866972987	0.866972987
f_9	1.15469	1.15469	1.1547049	1.1546961	1.154702007	1.154700538

In order to numerically evaluate the definite integral $I_a^b(f) = \int_a^b f(x) dx$, we take the simplest example of a straight line interpolating $f(x)$ at the endpoints of the interval. A linear interpolating polynomial is

$$p(x) = f(a) + (x - a) \frac{f(b) - f(a)}{b - a},$$

and after integration we obtain the *basic trapezoidal rule*:

$$I_a^b(f) \approx \int_a^b p(x) dx = \frac{b-a}{2} [f(a) + f(b)], \quad (2.5.1)$$

A better approximation is obtained by using an interpolating polynomial of higher degree. Thus, a quadratic interpolating polynomial which interpolates $f(x)$ at the

points a , $\frac{a+b}{2}$, and b is defined by

$$p(x) = f(a) + (x-a)f\left[a, \frac{a+b}{2}\right] + \left(x - \frac{a+b}{2}\right)(x-a)f\left[a, \frac{a+b}{2}, b\right],$$

and yields the *basic Simpson's rule*:

$$I_a^b(f) \approx S(f) = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]. \quad (2.5.2)$$

The basic Simpson's rule is three-point and has degree 3, although we started with fitting f by a quadratic. This feature makes Simpson's rule more accurate and widely used.

Now, we will further analyze the Simpson's rule $S(f)$. Let $c = \frac{a+b}{2}$, and split the integral into two parts:

$$I_a^b(f) = \int_a^c f(x) dx + \int_c^b f(x) dx.$$

Applying the integration by parts to each of these integrals, we get

$$\begin{aligned} I_a^b(f) &= [f(x)(x-c_1)]_{x=a}^c - \int_a^c f'(x)(x-c_1) dx, \\ \int_c^b f(x) dx &= [f(x)(x-c_2)]_{x=c}^b - \int_c^b f'(x)(x-c_2) dx, \end{aligned}$$

where c_1 and c_2 are arbitrary constants of integration. After adding these two expressions we obtain

$$\begin{aligned} I_a^b(f) &= f(b)(b-c_2) + f(c)(c_2-c_1) + f(a)(c_1-a) \\ &\quad - \int_a^c f'(x)(x-c_1) dx - \int_c^b f'(x)(x-c_2) dx. \end{aligned}$$

To obtain the Simpson's rule $S(f)$, we choose the values of c_1 and c_2 as

$$b-c_2 = \frac{b-a}{6}, \quad c_2-c_1 = \frac{4(b-a)}{6}, \quad c_1-a = \frac{b-a}{6}.$$

A unique solution of these three equations is

$$c_1 = \frac{5a+b}{6}, \quad c_2 = \frac{a+5b}{6}.$$

Define a function $g(x)$ by

$$g(x) = \begin{cases} x-c_1 & \text{if } a \leq x \leq c, \\ x-c_2 & \text{if } c < x \leq b. \end{cases}$$

Then we get

$$I_a^b(f) = S(f) - \int_a^b f'(x) g(x) dx, \quad (2.5.3)$$

provided $f \in C^1[a, b]$. If $|f'(x)| \leq M_1$ for $a \leq x \leq b$, then

$$\left| \int_a^b f(x) dx - S(f) \right| \leq M_1 \int_a^b |g(x)| dx.$$

Moreover, if $f \in C^4[a, b]$, then

$$I_a^b(f) = S(f) + \int_a^b f^{(4)}(x) k(x) dx, \quad (2.5.4)$$

where

$$k(x) = \begin{cases} \frac{(x-a)^3}{24} \left(x - \frac{a+2b}{3}\right) & \text{if } a \leq x \leq c, \\ \frac{(x-b)^3}{24} \left(x - \frac{2a+b}{3}\right) & \text{if } c < x \leq b. \end{cases}$$

The error in approximating the integral $I_a^b(f)$ by the Simpson's rule is given by

$$\left| I_a^b(f) - S(f) \right| = \frac{|b-a|^5}{2880} f^{(4)}(\xi), \quad a < \xi < b. \quad (2.5.5)$$

Note that since $k(x) < 0$ on $[a, b]$, we use the mean value theorem for integration and write

$$\int_a^b f^{(4)}(x) k(x) dx = f^{(4)}(\xi) \int_a^b k(x) dx,$$

and a simple calculation yields $\int_a^b k(x) dx = -\frac{(b-a)^5}{2880}$. The error bound (2.5.5) indicates that it may not be a good idea to apply the basic Simpson's rule to approximate the integral (2.5.1), because the length of the interval $|b-a|$ is raised to the fifth power. However, if we can reduce this length, we will reduce the error significantly. This is done by partitioning the interval $[a, b]$ into N equal subintervals of length $h = (b-a)/N$, and writing

$$I_a^b(f) = \sum_{i=0}^{N-1} \int_{a+ih}^{a+(i+1)h} f(x) dx.$$

Then applying the basic Simpson's rule to each integral, we obtain the repeated Simpson's rule:

$$\begin{aligned} I_a^b(f) &\approx S_N(f) \\ &= \sum_{i=0}^{N-1} \frac{h}{6} \left[f(a+ih) + 4f\left(a + (i+1/2)h\right) + f\left(a + (i+1)h\right) \right]. \end{aligned} \quad (2.5.6)$$

Alternatively, we use the Newton-Gregory forward polynomial (1.4.19) to integrate a function $f(x)$ with respect to x over an interval (a, b) . Thus,

$$\int_a^b f(x) dx \approx \int_a^b P_n(x_s) dx. \quad (2.5.7)$$

The error in this approximation is given by

$$E(x) = \int_a^b \binom{s}{n+1} h^{n+1} f^{(n+1)}(\xi) dx, \quad a < \xi < b. \quad (2.5.8)$$

If the interval of integration (a, b) matches the range of fit of the polynomial, which is (x_0, x_n) , i.e., when $a = x_0 < x_1 < x_2 < \dots < x_n = b$, then we obtain the *Newton-Cotes formulas*. These formulas are a set of integration rules which correspond to the varying degree of the interpolating polynomial. The first three Newton-Cotes formulas, with the degree of the polynomial as 1, 2, and 3, are especially important. They are:

$$\begin{aligned} n = 1 : \quad & \int_{x_0}^{x_1} f(x) dx \approx \int_{x_0}^{x_1} (f_0 + s\Delta f_0) ds = h \int_0^1 (f_0 + s\Delta f_0) dx \\ & = \frac{h}{2} (f_0 + f_1), \quad \text{where } s = (x - x_0)/h, dx = h ds, \end{aligned} \quad (2.5.9a)$$

$$\begin{aligned} \text{error} &= \int_{x_0}^{x_1} \binom{s}{2} h^2 f''(\xi) dx = \int_{x_0}^{x_1} \frac{s(s-1)}{2} h^2 f''(\xi) dx \\ &= \frac{h^3}{2} \int_0^1 s(s-1) f''(\xi) ds = -\frac{h^3}{12} f''(\xi), \quad x_0 < \xi < x_1; \end{aligned} \quad (2.5.9b)$$

$$\begin{aligned} n = 2 : \quad & \int_{x_0}^{x_2} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 \right) dx \\ &= h \int_0^2 \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 \right) ds \\ &= \frac{h}{3} (f_0 + 4f_1 + f_2), \end{aligned} \quad (2.5.10a)$$

$$\begin{aligned} \text{error} &= \int_{x_0}^{x_2} \frac{s(s-1)(s-2)(s-3)}{24} h^3 f^{iv}(\xi) dx \\ &= -\frac{1}{90} h^5 f^{iv}(\xi), \quad x_0 < \xi < x_2; \end{aligned} \quad (2.5.10b)$$

$$n = 3 : \quad \int_{x_0}^{x_3} f(x) dx = \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3), \quad (2.5.11a)$$

$$\text{error} = -\frac{3}{80} h^5 f^{iv}(\xi), \quad x_0 < \xi < x_3. \quad (2.5.11b)$$

Note that the error term for both $n = 2$ (quadratic) and $n = 3$ (cubic) cases is $O(h^5)$. Thus, the error of integration using a quadratic is the same as using a cubic. Also, the coefficient $-1/90$ in the quadratic case is smaller than the coefficient $-3/80$ in the cubic case, which means that the formula with $n = 2$ is more accurate than that with $n = 3$. In fact, this phenomenon is true for all even-order Newton-Cotes formulas; each has the same order of h in its error term as in the next higher (odd) order formula. This suggests that the even-order formulas are more useful for numerical integration.

The derivation of the class of Newton-Cotes (N-C) rules, where the nodes are equally spaced, is based on the use of the complete set of monomials $\{1, x, \dots, x^n\}$ for $f(x)$ for some n , which generate sufficient equations to evaluate and fix the sets w_k and x_k . The trapezoidal and Simpson's rules, among others, are special cases of the N-C rules (see §2.6.3). For implementation of the trapezoidal and Simpson's rules, see [trapsimp.f90](#), [trapsimp.m](#) and [trapsimp.nb](#) on the CD-R.

EXAMPLE 2.5.2. Using the test functions $f_1(x) = e^{-x}$, $f_2(x) = \cos x$, $f_3(x) = \sqrt{x}$, $f_4(x) = \frac{1}{1+x^2}$, $f_5(x) = \frac{1}{1+e^x}$, with $[a, b] = [0, 1]$ and $h = 1/40$, the basic rules yield the results presented in Table 2.5.2. ■

Table 2.5.2.

f	$R_n^{(1)}$	$R_n^{(2)}$	M_n	T_n	Simpson's	Exact
f_1	0.6400	0.6243	0.632104	0.63215348	0.63212056	0.63212056
f_2	0.8472	0.8357	0.841493	0.84142716	0.84147099	0.84147098
f_3	0.6534	0.6784	0.666894	0.66587096	0.66634576	0.66666667
f_4	0.7916	0.7791	0.785411	0.78537212	0.78539816	0.78539816
f_5	0.3828	0.3770	0.379884	0.37988827	0.37988549	0.37988549

2.6. Repeated Quadrature Rules

A quadrature rule $Q(f)$ is defined as

$$I_a^b(f) = \sum_{k=0}^n w_k f(x_k) + E(f), \quad (2.6.1)$$

where w_k are the weights (or coefficients) and x_k are the quadrature points (or base points or nodes). The interval $[a, b]$ is a finite or infinite interval of integration. The error term $E(f) = 0$ iff $f(x)$ is a polynomial of degree $\leq n$. Let the interval $[a, b]$ be finite and partitioned by n equally spaced points $x_k = a + kh$, $k = 0, 1, \dots, n$, where $h = (b - a)/n$. Sometimes we will use the notation: $f_k = f(x_k)$. The repeated quadrature rules are as follows:

\bar{R}_n : Repeated Rectangle Rule: $I_a^b \equiv \int_{x_0}^{x_n} f(x) dx \approx h \sum_{k=0}^n f(x_k)$.

M_n : Repeated Midpoint Rule: $I_a^b(f) = \int_{x_0}^{x_n} f(x) dx \approx h \sum_{k=0}^{n-1} F(a + (k + 1/2)h)$.

T_n : Repeated Trapezoidal Rule: $I_a^b(f) = \int_{x_0}^{x_n} F(s) ds \approx \frac{h}{2} \sum_{j=1}^{n+1} \{2f(x_k)\}$.

A generalization of the repeated trapezoidal rule is known as the *Gregory formula*:

$$\int_{x_0}^{x_N} f(x) dx = h(f_0 + f_1 + 2f_2 + \cdots + f_N) + h \sum_{j=0}^m c_{j+1} \left\{ \nabla^j f_N + (-1)^j \Delta^j f_0 \right\}, \quad (2.6.2)$$

where

$$c_j = (-1)^j \int_{-1}^0 \binom{-s}{j} ds.$$

This formula reduces to the repeated trapezoidal rule for $m = 0$. All values of c_j are negative. Some values of c_j are: $c_1 = -1/2$, $c_2 = -1/12$, $c_3 = -1/24$, $c_4 = -19/720$, $c_5 = -3/160$, $c_6 = -863/60480$, $c_7 = -275/24192$, $c_8 = -33953/3628800$, $c_9 = -8183/1036800$, $c_{10} = -3250433/479001600$. If $m \leq N$, the Gregory formula uses the values $f(x_i)$ for every $x_i \in [x_0, x_N]$. If $m = 2k$ (even) or $m = 2K + 1$ (odd), the Gregory formula has an error of order h^{m+2} . However, it provides an exact integration for all polynomials of degree $2k + 1$. For example, if $m = 2$ and $N \geq 2$, the Gregory formula is

$$\begin{aligned} \int_{x_0}^{x_N} f(x) dx &\approx h(f_0 + f_1 + 2f_2 + \cdots + f_N) - \frac{5h}{8}(f_0 + f_N) \\ &\quad + \frac{h}{6}(f_1 + f_{N-1}) - \frac{h}{24}(f_2 + f_{N-2}), \end{aligned} \quad (2.6.3)$$

which is exact if f is a polynomial of degree 3.

S_n : Repeated Simpson's rule:

$$\begin{aligned} I_a^b(f) = \int_{x_0}^{x_{2n}} f(x) dx &= \frac{h}{3} \left[f(x_0) + 4f(x_2) + 2f(x_4) + 4f(x_6) \right. \\ &\quad \left. + 2f(x_8) + \cdots + 4f(x_{2n-2}) + 2f(x_{2n}) \right]. \end{aligned}$$

The coefficients in this rule follow the pattern: 1 2 4 2 4 ... 2 4 2 4 1.

W_n : Repeated Weddle's rule:

$$I_a^b(f) = \int_{x_0}^{x_n} f(x) dx = \frac{3h}{10} \left[f(x_0) + 5f(x_1) + f(x_2) + 6f(x_3) + f(x_4) \right. \\ \left. + 5f(x_5) + 2f(x_6) + 5f(x_7) + f(x_8) + 6f(x_9) \right. \\ \left. + f(x_{10}) + \cdots + f(x_{n-2}) + f(x_{n-1}) + f(x_n) \right].$$

For $n = 6$ it reduces to the basic Weddle's rule.

\bar{T}_n : Repeated Tangent Rule:

$$\int_a^b f(x) dx \approx h \sum_{k=0}^n f(x_k),$$

where $x_k = a + kh/2$, with $x_n = b$. Details of some of these repeated rules are given below.

The trapezoidal rule is generally applied in its repeated (or composite) form T_n . Assuming that $f \in C^2[a, b]$ and taking $h = (b - a)/n$, we rewrite $T_n(f)$ as

$$T_n(f) = \frac{h}{2} (f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n) - \frac{nh^3}{12} f''(\xi), \quad (2.6.4)$$

$$= h(f_0 + f_1 + 2f_2 + \cdots + f_{n-1}) + \frac{h}{2} (f_n - f_0) \\ - (x_n - x_0) \frac{h^2}{12} f''(\xi), \quad (2.6.5)$$

where $a < \xi < b$, and $x_n - x_0 = nh$. Note that the repeated trapezoidal rule T_n consists of the repeated rectangle rule \bar{R}_n plus a correction term $\frac{h}{2} (f_n - f_0)$. The error term in (2.6.5) is of order h^2 and this rule is exact for all polynomials of degree one, because the second derivative in the error term is zero for such polynomials.

The rounding error on f_k does not seriously affect the accuracy of the quadrature rule. Suppose that the rounding error in f_k is at most $\frac{1}{2} \times 10^{-k}$. Then from the rule (2.6.4) we get

$$\frac{h}{2} (1 + 2 + 2 + \cdots + 2 + 1) \times \frac{1}{2} \times 10^{-k} = nh \times 10^{-k} = \frac{1}{2} (b - a) 10^{-k}.$$

We use the Newton-Gregory forward polynomial (1.4.19) with $n = 3$ and integrate $f(x)$ over $[x_0, x_2]$. This gives

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3} (f_0 + 4f_1 + f_2) - \frac{h^3}{90} f^{(4)}(\xi), \quad x_0 < \xi < x_2.$$

This is known as basic Simpson's rule. The repeated Simpson's rule requires an even number of subintervals.

2.6.1. An Initial Value Problem. The above quadrature rules contain the weighted sum of the values $w_i f(x_i)$, where the nodes x_i lie within the interval of integration $[a, b] \equiv [x_0, x_n]$. However, sometimes we run into the problem of integrating a function $f(x)$ over an interval $[x_0, x_{n+1}]$, where $x_n = x_0 + nh$, and the only known values of f are those at x_0, \dots, x_n . In such a situation we proceed as follows. Assuming that we have already computed the approximations at $x = x_n, x_{n-1}, \dots, x_{n-m}$ for $m \leq n$, we use the backward difference formulas (1.3.15) and (1.3.16) and obtain for any $s > 0$

$$f(x_n + sh) = \sum_{j=0}^m (-1)^j \binom{-s}{j} \nabla^j f_n + (-1)^{m+1} h^{m+1} \binom{-s}{m+1} f^{(m+1)}(\xi_s), \quad (2.6.6)$$

where $x_{n-m} < \xi_s < x_n + sh$, and $f^{(m+1)}$ is continuous on $[x_{n-m}, x_n + sh]$. Now, we integrate (2.6.6) over the interval $[x_n, x_{n+1}]$ by setting $x = x_n + sh$, and obtain

$$\begin{aligned} \int_{x_n}^{x_{n+1}} f(x) dx &= h \sum_{j=0}^m (-1)^j \nabla^j f_n \int_0^1 \binom{-s}{j} ds \\ &\quad + (-1)^{m+1} h^{m+2} \int_0^1 \binom{-s}{m+1} f^{(m+1)}(\xi_s) ds \\ &= h \sum_{j=0}^m b_j \nabla^j f_n \int_0^1 \binom{-s}{j} ds + h^{m+2} b_{m+1} f^{(m+1)}(\xi_s), \end{aligned} \quad (2.6.7)$$

where

$$b_j = (-1)^j \int_0^1 \binom{-s}{j} ds, \quad (2.6.8)$$

and $x_{n-m} < \xi_s < x_{n+1}$.

Another method is to use $f(x_{n+1})$ and construct the interpolating polynomial at the points $x = x_{n+1}, x_n, \dots, x_{n-m}$ for $m \leq n$. In this case we obtain

$$\begin{aligned} f(x_{n+1} + sh) &= \sum_{j=0}^{m+1} (-1)^j \binom{-s}{j} \nabla^j f_{n+1} \\ &\quad + (-1)^{m+2} h^{m+2} \binom{-s}{m+2} f^{(m+2)}(\xi_s). \end{aligned} \quad (2.6.9)$$

Note that the interval $x_n \leq x \leq x_{n+1}$ corresponds to $-1 \leq s \leq 0$. Using the fundamental theorem of integral calculus we get

$$\int_{x_n}^{x_{n+1}} f(x) dx = h \sum_{j=0}^{m+1} c_j \nabla^j f_{n+1} + h^{n+3} c_{m+2} f^{(m+2)}(\eta_s), \quad (2.6.10)$$

where $x_{n-m} < \eta_s < x_{n+1}$, and c_j are defined by (2.6.2).

EXAMPLE 2.6.1. We consider the problem of integrating a first-order initial value problem involving the ordinary differential equation $y' = f(x)$ between the limits x_n and x_{n+1} . The numerical solution is given by

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x)) dx. \quad (2.6.11)$$

The integral in (2.6.11) can be numerically solved, for example, by replacing the integral by an interpolating polynomial. Suppose we have already computed the approximations y_0, y_1, \dots, y_n at the nodes $x_k = x_0 + kh$, $k = 0, 1, \dots, n$. Now, to approximate the integrand $f(x, y(x))$ between x_n and x_{n+1} we construct an interpolating polynomial $p_m(x)$ through the $m+1$ points $(x_n, f_n), (x_{n-1}, f_{n-1}), \dots, (x_{n-m}, f_{n-m})$, where $m \leq n$. This replaces (2.6.11) by

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} p_m(x) dx. \quad (2.6.12)$$

Using the backward difference formula (1.3.15) we get

$$p_m(x) = \sum_{j=0}^m (-1)^j \binom{-s}{j} \nabla^j f_n.$$

Thus,

$$\int_{x_n}^{x_{n+1}} f(x, y(x)) dx \approx \int_{x_n}^{x_{n+1}} p_m(x) dx = h \sum_{j=0}^m b_j \nabla^j f_n, \quad (2.6.13)$$

where b_j , defined by (2.6.8), are independent of both m and n . Some values of the coefficient b_j are: $b_0 = 1$, $b_1 = 1/2$, $b_2 = 5/12$, $b_3 = 3/8$, and $b_4 = 251/720$. Hence, from (2.6.12) and (2.6.13) we find the solution as

$$y_{n+1} = y_n + h \sum_{j=0}^m b_j \nabla^j f_n \quad \text{for } n = m, m+1, \dots \quad (2.6.14)$$

This is known as the *Adams-Bashforth formula* for the initial value problem (2.6.11).

If we expand the differences in (2.6.14), the solution reduces to

$$y_{n+1} = y_n + h \sum_{j=0}^m \beta_j f_{n-j}, \quad (2.6.15)$$

where β_j depend on m . For example, for $m = 1$ we have $y_{n+1} = y_n + \frac{h}{2} (3f_n - f_{n-1})$, and for $m = 3$ we get

$$y_{n+1} = y_n + \frac{h}{24} (55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}). \quad \blacksquare$$

The *Adams-Bashforth algorithm* of order 4 (i.e., $m = 3$) is

1. Choose a step size h such that $(b - a)/h$ is an integer.

2. Start with y_0, y_1, y_2, y_3 .

$$X := a + 3h; \quad Y := y_3$$

$$F_0 := f(X, y_3)$$

$$F_1 := f(X - h, y_2)$$

$$F_2 := f(X - 2h, y_1)$$

$$F_3 := f(X - 3h, y_0)$$

repeat

$$Y := Y + \frac{h}{24} (55F_0 - 59F_1 + 37F_2 - 9F_3)$$

$$F_3 := F_2; \quad F_2 := F_1; \quad F_1 := F_0$$

$$X := X + h$$

$$F_0 := f(X, Y)$$

until $X = b$

The local truncation error in the Adams-Bashforth formula is given by

$$E_{\text{Local}} = h^{m+1} b_{m+1} y^{(m+1)}(\xi_n), \quad x_{n-m} < \xi_n < x_{n+1}. \quad (2.6.16)$$

The global truncation error in this formula is bounded by

$$E_{\text{Global}} \leq \frac{h^{m+1} |b_{m+1}| M_{m+2}}{L B_m}, \quad (2.6.17)$$

where $\max_{x \in [x_0, b]} |y^{(m+2)}(x)| \leq M_{m+2}$, $B_m = |\beta_0| + |\beta_1| + \cdots + |\beta_m|$, and L is the Lipschitz constant such that $|f(x_n, y(x_n)) - f(x_n, y_n)| \leq L |y(x_n) - y_n|$. The bound in (2.6.17) is, however, of qualitative interest and does not provide any computationally useful information. For an implementation of this method, see [AdamsBashforth.m](#) on the CD-R.

EXAMPLE 2.6.2. Solve $y' = \frac{1}{1+y^2}$, $y(0) = 1$, and $0 \leq x \leq 1$. We have $f(x, y) = \frac{1}{1+y^2}$, and by the mean value theorem $f(x, y) - f(x, z) = (y - z) \frac{\partial f(x, \xi)}{\partial y}$, where ξ lies between y and z . To satisfy the Lipschitz condition $|f(x, y) - f(x, z)| \leq L |y - z|$, we choose $L \geq \left| \frac{\partial f(x, y)}{\partial y} \right| = \left| \frac{-2y}{(1+y^2)^2} \right|$ for all $x \in [0, 1]$ and $y \in (-\infty, \infty)$. Since a maximum for $\frac{2y}{(1+y^2)^2}$ occurs at $y = \pm \frac{1}{\sqrt{3}}$, we take $L = \left| \frac{\partial f(x, 1/\sqrt{3})}{\partial y} \right| = \frac{3\sqrt{3}}{8}$. Now, since $f''(x, y) = \frac{2(5y^2 - 1)}{(1+y^2)^3}$, we find that

$$|y''(x)| = |f''(x, y(x))| \leq \left| \frac{10y^2 - 2}{(1+y^2)^3} \right| = 2.$$

Thus, we choose $M = 2$. For the Adams-Bashforth formula of order 2, we have $m = 1$, $b_2 = 5/12$, $B_1 = |\beta_0| + |\beta_1| = 2$, and thus, from (2.6.17) we have

$$\begin{aligned} |y(x_n) - y_n| &\leq \left\{ \delta + h^2 \frac{5}{12} \cdot \frac{8}{3\sqrt{3}} \cdot \frac{2}{2} \right\} e^{3\sqrt{3}(x_n-0)/4} - h^2 \frac{5}{12} \cdot \frac{8}{3\sqrt{3}} \cdot \frac{2}{2} \\ &= \left(\delta + \frac{10h^2}{9\sqrt{3}} \right) e^{3\sqrt{3}x_n/4} - \frac{10h^2}{9\sqrt{3}}, \end{aligned}$$

where $\delta = \max_{0 \leq k \leq m} |y(x_k) - y_k|$. Then by taking $h = 0.1$, $n = 10$, and $\delta = 10^{-5}$, we get $|y(1.0) - y_{10}| \leq 0.0172$. This bound is considerably larger, because the values of $y(1.0) = 1.40629$ and $y_{10} = 1.40584$ yield $|y(1.0) - y_{10}| = 0.00045$. The local truncation error is $E_{\text{Local}} = h^2 b_2 y'''(\xi_n) = (0.1)^2 \cdot \frac{5}{12} \cdot (2.403486046) = 0.010014525$. ■

2.7. Romberg's Scheme

The classical Romberg scheme is a numerical integration procedure that amounts to using the Richardson extrapolation (§1.4.4) on the repeated trapezoidal rule. This scheme improves the accuracy in the Newton-Cotes formulas. This method is based on the trapezoidal rule which is written as

$$\int_a^b f(x) dx = h \sum_{j=0}^n f_j + \sum_{i=1}^{\infty} a_i h^{2i}. \quad (2.7.1)$$

where $h = (b - a)/n$, and a_k depend only on a , b , and $f(x)$. Let

$$I = \int_a^b f(x) dx,$$

and

$$T_{0,k} = \frac{b-a}{2^k} \left(\frac{1}{2} f_0 + f_1 + f_2 + \cdots + f_{2^k-1} + \frac{1}{2} f_{2^k} \right) \quad (2.7.2)$$

denote the trapezoidal rule for 2^k subintervals of $[a, b]$. Then

$$T_{0,k} = I - \sum_{i=1}^{\infty} a_i \left(\frac{b-a}{2^k} \right)^{2i}. \quad (2.7.3)$$

Define

$$T_{1,k} = \frac{1}{3} (4T_{0,k+1} - T_{0,k}), \quad k = 0, 1, \dots \quad (2.7.4)$$

Then, using (2.7.3) we get

$$\begin{aligned} T_{1,k} &= I - \sum_{i=1}^\infty \frac{1}{3} \left(\frac{4}{2^{2i}-1} \right) a_i \left(\frac{b-a}{2^k} \right) \\ &= I - \sum_{i=2}^\infty \frac{1}{3} \left(\frac{4}{2^{2i}-1} \right) a_i \left(\frac{b-a}{2^k} \right), \quad k = 0, 1, \dots \end{aligned} \tag{2.7.5}$$

The approximation $T_{1,k}$ is known as the *parabolic rule* for 2^k subintervals. This rule approximates I using step sizes $h_1 = (b-a)/2^{k+1}$ and $h_2 = (b-a)/2^k$, and has a leading term with the error of the order h_2^4 . Thus, in general, we define

$$T_{m,k} = \frac{1}{4^m - 1} \left(4^m T_{m-1,k+1} - T_{m-1,k} \right), \quad k = 0, 1, \dots \quad m = 1, 2, \dots \tag{2.7.6}$$

This is known as the *Romberg formula*. Each $T_{m,k}$ is a linear combination of trapezoidal rules using $2^k, 2^{k+1}, \dots, 2^{2k}$ subintervals. Note that the approximation $T_{2,k}$ defines the composite rule using the Newton-Cotes closed formula for $n = 4$ and 2^k subintervals. However, for $m > 2$ the rule (2.7.6) has no direct connection with a Newton-Cotes repeated (composite) rule. The computations for $T_{m,k}$ can be arranged in the form of Table R.1.

Table R.1. Romberg Table.

$T_{0,0}$					
$T_{0,1}$	$T_{1,0}$				
$T_{0,2}$	$T_{1,1}$	$T_{2,0}$			
\vdots	\vdots		\ddots		
\vdots	\vdots			\ddots	
$T_{0,m}$	$T_{1,m-1}$	\dots	\dots	\dots	$T_{m,0}$

In the first column we use $m + 1$ computations of the trapezoidal rule and then use formula (2.7.6) to compute all the remaining entries in the above table. If f is Riemann-integrable in $[a, b]$, then $T_{0,m} \rightarrow I$ as $m \rightarrow \infty$. Note that $T_{m,k}$ has the leading term in its error of order of $((b-a)/2^k)$, while $T_{0,k}$ has the leading term in its order of $((b-a)/2^k)^2$. Thus, we can hope that $T_{m,k}$ converges much faster than $T_{0,k}$.

We can write the Romberg formula (2.7.6) in the form

$$T_{m,k} = \sum_{j=0}^m c_{m,m-j} T_{0,k+j}, \tag{2.7.7}$$

which leads to the matrix equation

$$\begin{Bmatrix} T_{0,0} \\ T_{1,0} \\ \vdots \\ T_{m,0} \end{Bmatrix} = \begin{bmatrix} c_{00} & & & \\ c_{11} & c_{10} & & \\ \vdots & & \ddots & \\ c_{mm} & \cdots & \cdots & c_{m0} \end{bmatrix} \begin{Bmatrix} T_{0,0} \\ T_{0,1} \\ \vdots \\ T_{0,m} \end{Bmatrix}. \quad (2.7.8)$$

The coefficients c_{mj} are the coefficients of

$$t_m(z) = \sum_{j=0}^m c_{mj} z^j = \frac{(4-z)(4^2-z)\cdots(4^m-z)}{(4-1)(4^2-1)\cdots(4^m-1)}, \quad (2.7.9)$$

In particular, we have

$$\sum_{j=0}^m |c_{mj}| = \prod_{j=1}^m \frac{4^j + 1}{4^j - 1} < \prod_{j=1}^{\infty} \frac{4^j + 1}{4^j - 1}. \quad (2.7.10)$$

Since this infinite product converges, the sum of magnitudes of elements in any row of (2.7.8) is bounded. We find (2.7.9) that $c_{m,m-j} \rightarrow 0$ as $m \rightarrow \infty$, which implies that each column in (2.7.8) converges to zero. Finally, $\sum_{j=0}^m c_{mj} = t_m(1) = 1$. Thus, the coefficient matrix in (2.7.8) satisfies the conditions for Toeplitz convergence; i.e., $T_{0,m}$ as well as $T_{m,0}$ converges to I .

The Romberg method is based on the convergence of the above procedure which is an extension of the Richardson extrapolation and deals with performing M computations, each using a different value of h , and then eliminating the first $M - 1$ terms in the error term in (2.7.3). The convergence in this procedure occurs only in the case of the trapezoidal rule (see [Ralston-Rabinowitz](#), pp.123-124).

A simplified version is as follows (Phillips and Taylor 1996, pp.169). The Simpson's rule can be expressed as a linear combination of the midpoint and trapezoidal rules by

$$S(h/2) = \frac{4T(h/2) - T(h)}{3}. \quad (2.7.11)$$

Let $f \in C^\infty[a, b]$. Then, using the Euler-Maclaurin formula (2.2.8), we can write

$$I - T(h) = h^2 E_2 + h^4 E_4 + h^6 E_6 + \cdots, \quad (2.7.12)$$

where $h = (b - a)/n$ and

$$E_{2k} = -\frac{B_{2k}}{(2k)!} \left(f^{(2k-1)}(b) - f^{(2k-1)}(a) \right),$$

and the coefficients B_{2k} are the Bernoulli numbers (§2.2.2). If h in (2.7.12) is replaced by $h/2$, which doubles the number of subintervals, we obtain

$$I - T\left(\frac{h}{2}\right) = \left(\frac{h}{2}\right)^2 E_2 + \left(\frac{h}{2}\right)^4 E_4 + \left(\frac{h}{2}\right)^6 E_6 + \cdots. \quad (2.7.13)$$

Now we eliminate the h^2 term between (2.7.12) and (2.7.13) by multiplying (2.7.13) by 4, subtracting (2.7.12) and dividing by 3. This leads to

$$I - T^{(1)}(h) = h^4 E_4^{(1)} + h^6 E_6^{(1)} + \cdots, \quad (2.7.14)$$

where

$$T^{(1)}(h) = S(h/2),$$

as defined by (2.7.11), and $E_4^{(1)}, E_6^{(1)}, \dots$ are multiples of E_4, E_6, \dots . Note that $T^{(1)}(h)$, defined by (2.7.14), provides a better approximation to the integral I for sufficiently small values of h than provided by either the trapezoidal rule $T(h)$ or $T(h/2)$.

The above process of eliminating the leading power of h in the error term is the Richardson extrapolation (see §1.4.4). If we continue this process further, eliminating terms in h^4 between $T^{(1)}(h)$ and $T^{(1)}(h/2)$, we obtain

$$I - T^{(2)}(h) = h^6 E_6^{(2)} + h^8 E_8^{(2)} + \cdots,$$

where

$$T^{(2)}(h) = \frac{16T^{(1)}(h/2) - T^{(1)}(h)}{15}, \quad (2.7.15)$$

where the numbers $E_6^{(2)}, E_8^{(2)}, \dots$ are multiples of $E_6^{(1)}, E_8^{(1)}, \dots$, and hence, multiples of E_6, E_8, \dots . In general, continuing this process to k steps further, we obtain

$$I - T^{(k)}(h) = h^{2(k+1)} E_{2(k+1)}^{(k)} + \cdots, \quad (2.7.16)$$

where

$$T^{(k)}(h) = \frac{4^k T^{(k-1)}(h/2) - T^{(k-1)}(h)}{4^k - 1}. \quad (2.7.17)$$

This is the *Romberg formula*. To compute $T^{(k)}(h)$ we need to compute the trapezoidal approximations $T(h), T(h/2), T(h/4), \dots, T(h/2^k)$. This can be arranged in the form of Table R.2 which is designed for $k = 3$.

Table R.2. Romberg Table.

$T(h)$	$T^{(1)}(h)$	$T^{(2)}(h)$	$T^{(3)}(h)$
$T(h/2)$	$T^{(1)}(h/2)$	$T^{(2)}(h/2)$	
$T(h/4)$	$T^{(1)}(h/4)$		
$T(h/8)$			

EXAMPLE 2.7.1. (Phillips and Taylor 1996, p. 171) Apply the Romberg formula to compute the integral $\int_0^1 \frac{dx}{1+x}$ with $n = 1$ and $k = 3$. The correct result to six

decimal places is 0.693155 (Mathematica value is 0.693147). Note that $0.25 \leq f(x) \leq 2$ for $0 \leq x \leq 1$. Applying the above algorithm we obtain the answer as 0.693148 (see Table 2.7.1). ■

Table 2.7.1.

0.750000	0.694444	0.693175	0.693148
0.708333	0.693254	0.693148	
0.697024	0.693155		
0.694122			

EXAMPLE 2.7.2. (Phillips and Taylor 1996, p. 172.) Compute $\int_0^{0.8} \sqrt{x} dx$. The value correct to six decimal figures is 0.47703 (Mathematica value is 0.477028). The integrand is not differentiable at $x = 0$. We take $h = 0.8/2^n$ for $n = 0, 1, 2, 3, 4$, and the results using the above algorithm are presented in Table 2.7.2. Note that the two boxed values are not correct.

Table 2.7.2.

0.35777	0.45657	0.47066	0.47484	0.47626
0.43187	0.46978	0.47477	0.47625	
0.46030	0.47446	0.47623		
0.47092	47612			
0.47482				

Note that just looking at the last entries of the columns may not give us the correct result. We should look for the signs of convergence as we look down each column in the Romberg table of extrapolated values. ■

EXAMPLE 2.7.3. (Gerald and Weatley 1994, p. 334) Compute $I = \int_{0.2}^{1.5} e^{-x^2} dx$ (Mathematica value is 0.658823). By taking $h = (b - a)/2 = 0.65$, the first estimate is

$$I = \frac{h}{2} [f(a) + 2f(a + h) + f(b)] = \frac{0.65}{2} [e^{-0.2^2} + 2e^{-0.85^2} + e^{-1.5^2}] = 0.66211.$$

For the next estimate we take $h = 0.65/2 = 0.325$ and get

$$\begin{aligned} I &= \frac{h}{4} [f(a) + 2f(a + h) + 2f(a + 2h) + 2f(a + 3h) + f(b)] \\ &= \frac{0.325}{2} [e^{-0.2^2} + 1e^{-0.525^2} + 2e^{-0.85^2} + 2e^{-1.175^2} + e^{-1.5^2}] \\ &= 0.65947. \end{aligned}$$

Now we extrapolate to obtain

$$\text{Improved Value} = 0.65947 + \frac{0.65947 - 0.66211}{3} = 0.65859.$$

This process continues until the values finally match. This is shown in Table 2.7.3 as the boxed value. ■

Table 2.7.3.

0.66211	0.65859	0.65882	<div>0.65882</div>
0.65947	0.65881	0.65882	
0.65898	0.65882		
0.65886			

EXAMPLE 2.7.4. (Gerald and Weatley 1994, p. 335) Consider the function $f(x)$ tabulated in Table 2.7.4a.

Table 2.7.4a.

x	$f(x)$	x	$f(x)$
1.6	4.953	2.8	16.445
1.6	6.050	3.0	20.086
2.0	7.389	3.2	24.533
2.2	9.025	3.4	29.964
2.4	11.023	3.6	36.598
2.6	13.464	3.8	44.701

Compute the integral of this $f(x)$ between the limits $x = 1.8$ and $x = 3.4$. For $h = 0.2$ the first estimate is

$$\begin{aligned} I &= \frac{0.2}{2} [6.050 + 2(7.389) + 2(9.025) + 2(11.023) + 2(13.464) \\ &\quad + 2(16.445) + 2(20.086) + 2(24.533) + 29.964] \\ &= 23.9944. \end{aligned}$$

Now we take $h = 0.4$, which gives the next estimate as

$$\begin{aligned} I &= \frac{0.4}{2} [6.050 + 2(9.025) + 2(13.464) + 2(20.086) + 29.964] \\ &= 24.2328. \end{aligned}$$

Using extrapolation we get

$$\text{Improved Value} = 23.9944 + \frac{23.9944 - 24.2328}{3} = 23.9149.$$

The results of this process are shown in Table 2.7.4b.

Table 2.7.4b.

$h = 0.2$	23.9944	23.9149	23.9147
$h = 0.4$	24.2328	23.9181	
$h = 0.8$	25.1768		

EXAMPLE 2.7.5. (Kythe and Wei 2004, p. 72; Bickford 1990, p. 184) Solve by using the method of finite elements the heat transfer problem:

$$-\frac{d}{dx} \left(kA \frac{dT}{dx} \right) + \beta p T = qA, \quad 0 < x < L,$$

subject to the boundary conditions $T(0) = T_0$ and $T(L) = 0$ for a circular bar whose radius varies linear from r_0 at $x = 0$ to $r_0/4$ at $x = L$ (see Fig. 2.7.1, page 540), where $A(x) = A_0 \left(1 - \frac{3x}{4L}\right)^2$, $A_0 = \pi r_0^2$, and $p(x) = p_0 \left(1 - \frac{3x}{4L}\right)$, $p_0 = 2\pi r_0$, by taking a mesh of 2, 4, 8, 16 and 32 equally-spaced linear elements. We take $u = T/T_0$, $s = x/L$. Then the problem reduces to the nondimensional form

$$-\frac{d}{ds} \left[\left(1 - \frac{3s}{4}\right)^2 \frac{du}{ds} \right] + (cL)^2 \left(1 - \frac{3s}{4}\right) u = QL^2 \left(1 - \frac{3s}{4}\right)^2, \quad 0 < s < 1,$$

$$u(0) = 1, \quad u(1) = 0,$$

where $c^2 = \frac{\beta p_0}{kA_0}$, and $Q = \frac{q}{k}$.

We will improve the value of $u(0.5)$ by using the Romberg method. The Romberg table is presented in Table 2.7.5, in which the second column shows the values of $u(0.5)$ for the type of mesh mentioned in the first column. The extrapolation is carried out in the remaining columns. ■

Table 2.7.5: Extrapolation for the Values of $u(0.5)$.

2-Element Mesh:	0.757314	0.774057	0.776890	0.776447	0.776476
4-Element Mesh:	0.769871	0.776182	0.776558	0.776476	
8-Element Mesh:	0.774604	0.776464	0.776497		
16-Element Mesh:	0.775999	0.776488			
32-Element Mesh:	0.776366				

Since Romberg integration is an extrapolation problem, one must be careful in the application of this scheme.

2.8. Gregory's Correction Scheme

If $f(x)$ is sufficiently differentiable with respect to $x \in [a, b]$, a deferred correction is used to obtain the approximate solution I by using Gregory's correction. Suppose that an initial approximation $I = I^{(0)}$ is found after using a quadrature rule, say a repeated trapezoidal rule with step size $h = (b - a)/n$. Then we should compute only the vector $\mathbf{I}_h^{(0)} = [I^{(0)}(a), I^{(0)}(a + h), \dots, I^{(0)}(b)]^T$, where

$$\mathbf{I}_h^{(0)}(a + ih) - \lambda h \sum_{j=0}^n {}''k(a + ih, a + jh) \mathbf{I}_h^{(0)}(a + jh) = f(a + ih), \quad (2.8.1)$$

for $i = 0, 1, \dots, n$ (compare this with the repeated trapezoidal rule). If we use Gregory's method instead of the repeated trapezoidal rule, we get

$$\mathbf{I}_h(a + ih) - \lambda \left\{ h \sum_{j=0}^n {}''k(a + ih, a + jh) \mathbf{I}_h(a + jh) + \delta_i(\mathbf{I}) \right\} = f(a + ih), \quad (2.8.2)$$

for $i = 0, 1, \dots, n$, where $\delta_i(\mathbf{I})$ is Gregory's correction term to the repeated trapezoidal rule, defined by

$$\begin{aligned} \delta_i(\mathbf{I}) &= h \sum_{m=1}^p c_m^* \left\{ \nabla^m \vartheta_i(\mathbf{I}; b) + (-1)^m \Delta^m \vartheta_i(\mathbf{I}; a) \right\}, \quad p \leq n, \\ \nabla^m \vartheta_i(\mathbf{I}; b) &= \Delta^m \vartheta_i(x) \Big|_{x=b}, \\ \Delta^m \vartheta_i(\mathbf{I}; a) &= \Delta^m \vartheta_i(x) \Big|_{x=a}, \\ \vartheta_i(x) &= \vartheta_i(\mathbf{I}; x) = k(a + ih, x) \mathbf{I}(x). \end{aligned} \quad (2.8.3)$$

This method uses the forward and backward differences Δ^m and ∇^m , respectively, defined for $m \geq 1$ by

$$\begin{aligned} \Delta^m \vartheta(x) &= \Delta^{m-1} \vartheta(x + h) - \Delta^{m-1} \vartheta(x), \\ \nabla^m \vartheta(x) &= \Delta^m \vartheta(x - mh), \end{aligned}$$

such that

$$\Delta^m \vartheta(x) = \nabla^m \vartheta(x + mh) = \sum_{j=0}^m (-1)^{j+m} \binom{m}{j} \vartheta(x + jh),$$

coefficients c_m^* are defined by the recursive formula (see [Henrici 1964, p.252](#))

$$\begin{aligned} c_0^* &= 1, \\ c_m^* &= - \left[\frac{1}{2} c_{m-1}^* + \dots + \frac{1}{m+1} c_0^* \right], \quad m = 1, 2, \dots \end{aligned}$$

Some values of c_m^* are: $c_1^* = \frac{1}{2}$, $c_2^* = -\frac{1}{12}$, $c_3^* = -\frac{1}{24}$, $c_4^* = -\frac{19}{720}$, $c_5^* = -\frac{3}{160}$, $c_6^* = -\frac{863}{160480}$. Thus, we can write the trapezoidal rule with Gregory's correction as

$$\begin{aligned} I \approx & \frac{h}{2} \left[f(a) + 2f(a+h) + 2f(a+2h) + \dots + 2f(b-h) \right. \\ & \left. + f(b) \right] - \frac{h}{12} (\nabla f(b) - \Delta f(a)) - \frac{h}{24} (\nabla^2 f(b) - \Delta^2 f(a)) \\ & - \frac{19h}{720} (\nabla^3 f(b) - \Delta^3 f(a)) - \frac{3h}{160} (\nabla^4 f(b) - \Delta^4 f(a)) \\ & - \frac{863h}{60480} (\nabla^5 f(b) - \Delta^5 f(a)), \end{aligned} \quad (2.8.4)$$

and so on. For an application of this scheme to integral equations, see §10.3.

2.9. Interpolatory Product Integration

We will construct a quadrature rule for an integral with an integrand that is the product of any two functions $w(x)$ and $f(x)$ over an interval $[a, b]$. Such a rule is of the form

$$\int_a^b w(s)f(s) ds = \sum_{j=0}^n v_j f(s_j), \quad (2.9.1)$$

where s_j are the nodes, $a \leq s_j \leq b$, and the weights v_j depend on a, b as well as the function $w(x)$. If the function $w \equiv 1$, the rule (2.9.1) reduces to the quadrature rules presented in previous sections and [Chapter 3](#). We discuss two cases:

CASE 1. If the function $f(x)$ is “badly behaved”, e.g., $f(x)$ behaves like $(x - s)^{-1/2}$ near $x = s$ but is continuous everywhere else, we can find a function $g(x)$ such that $f(x) = g(x)(x - s)^{-1/2}$. In general, if we approximate $f(x)$ by using a polynomial interpolant

$$P_{0,1,\dots,n}(x) = \sum_{j=0}^n l_j(x) f(s_j),$$

where $l_j(x) = \prod_{\substack{i=0 \\ i \neq j}}^n \frac{x - s_i}{s_j - s_i}$, which agrees with $f(x)$ at the nodes s_j , $j = 0, 1, \dots, n$,

then

$$\int_a^b w(s)P_{0,1,\dots,n}(s) ds = \sum_{j=0}^n v_j f(s_j),$$

where $v_j = \int_a^b w(s) l_j(s) ds$. Since $f \in C[a, b]$, we choose the nodes s_0, s_1, \dots, s_n such that $P_{0,1,\dots,n}(x)$ is a reasonable approximation of $f(x)$.

EXAMPLE 2.9.1. Suppose $s_0 = a$, $s_1 = b$, and $f'' \in C[a, b]$. Then $l_0(x) = \frac{b-x}{b-a}$ and $l_1(x) = \frac{x-a}{b-a}$, which gives $P_{0,1,\dots,n}(x) = \frac{b-x}{b-a} f(a) + \frac{x-a}{b-a} f(b)$, and $\int_a^b w(s) f(s) ds = v_0 f(a) + v_1 f(b)$, where

$$v_0 = \int_a^b \frac{b-s}{b-a} w(s) ds, \quad v_1 = \int_a^b \frac{s-a}{b-a} w(s) ds. \blacksquare$$

CASE 2. For integral equations of the form $\int_a^b k(x, s) \phi(s) ds$, we keep x fixed, write $w(s) = k(x, s)$, and get an integral of the form (2.9.1), where the function $w(x)$ may be well behaved, or it may be badly behaved as, e.g., in the case of weakly singular integral equations where $w(s)$ may be of the form $|x-s|^{-\alpha} g(x, s)$, $0 < \alpha < 1$. If $\phi \in C^{n+1}[a, b]$, and $a \leq s_i \leq b$, $i = 0, 1, \dots, n$, then there is a value ξ depending on a such that

$$\phi(x) - P_{0,1,\dots,n}(x) = \frac{\phi^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^n (x - s_i).$$

Hence, in the case when a and b are finite,

$$\int_a^b w(s) \phi(s) ds - \int_a^b w(s) P_{0,1,\dots,n}(s) ds = \int_a^b w(s) \frac{\phi^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^n (s - s_i) ds,$$

where $\xi = \xi(s)$. If in (2.9.1) we set

$$v_j = \int_a^b w(s) \prod_{i \neq j} \frac{s - s_i}{s_j - s_i} ds,$$

then the error E in the above approximation is bounded by

$$|E| \leq \|\phi^{(n+1)}(x)\|_{\infty} \int_a^b \left| w(s) \prod_{i \neq j} \frac{s - s_i}{s_j - s_i} \right| ds, \quad (2.9.2)$$

provided $\int_a^b |w(s)| ds < \infty$. This leads to the quadrature rule

$$\int_a^b k(x, s) \phi(s) ds = \sum_{j=0}^n v_j \phi(s_j), \quad (2.9.3)$$

which is exact when $\phi(x) \in \mathcal{P}_n$.

To obtain an improved approximation, partition $[a, b]$ at the points s_j , $j = 0, 1, \dots, n$, by $a = s_0 < s_1 < \dots < s_n = b$, and write

$$\int_a^b w(s)f(s) ds = \sum_{j=0}^{n-1} \int_{s_j}^{s_{j+1}} w(s)f(s) ds = \sum_{j=0}^{n-1} \left\{ v_0^{(j)} f(s_j) + v_1^{(j)} f(s_{j+1}) \right\}, \quad (2.9.4)$$

where

$$\begin{aligned} v_0^{(j)} &= \int_{s_j}^{s_{j+1}} \frac{s_{j+1} - s}{s_{j+1} - s_j} w(s) ds, \\ v_1^{(j)} &= \int_{s_j}^{s_{j+1}} \frac{s - s_j}{s_{j+1} - s_j} w(s) ds. \end{aligned} \quad (2.9.5)$$

The approximation is still of the form (2.9.1), and the error is bounded by

$$|E| \leq \frac{1}{2} \|f''(x)\|_{\infty} \sum_{j=0}^n \int_{s_j}^{s_{j+1}} |w(s)(s - s_j)(s - s_{j+1})| ds,$$

which is of the order $O(h^2)$ at $s_j = a + jh$, $h = (b-a)/n$, provided $\int_a^b |w(s)| ds < \infty$. This quadrature is known as the GENERALIZED TRAPEZOIDAL RULE since it is an extension of the repeated trapezoidal rule. A GENERALIZED MIDPOINT RULE is obtained by taking n even and setting $s_j = a + jh$ as above, with $v_0 = v_2 = v_4 = \dots = 0$, and $v_{2m+1} = \int_{s_{2m}}^{s_{2m+2}} w(s)f(s) ds$ for $m = 0, 1, \dots$. This rule is exact if $f(x)$ is piecewise-constant, i.e., constant in each subinterval $[s_{2m}, s_{2m+2}]$. An extension of Simpson's rule is obtained for even n by setting $s_j = a + jh$, as above. Then in the subinterval $[s_{2m}, s_{2m+2}]$ the function $f(x)$ is approximated by the interpolant

$$\begin{aligned} P_{0,1,\dots,n}(x) &= \frac{1}{h^2} \left[\frac{1}{2} (x - s_{2m+1})(x - s_{2m+2}) f(s_{2m}) + (x - s_{2m})(x - s_{2m+2}) \right. \\ &\quad \left. \times f(s_{2m+1}) + \frac{1}{2} (x - s_{2m})(x - s_{2m+1}) f(s_{2m+2}) \right]. \end{aligned}$$

This gives the GENERALIZED SIMPSON'S RULE:

$$\int_a^b w(s)f(s) ds = \sum_{m=0}^{n/2-1} \int_{s_{2m}}^{s_{2m+2}} w(s)P_{0,1,\dots,n}(s) ds = \sum_{j=0}^n v_j f(s_j), \quad (2.9.6)$$

where

$$\begin{aligned}
 v_0 &= \frac{1}{2h^2} \int_a^{a+2h} (s-s_1)(s-s_2)w(s)ds, \\
 v_{2j+1} &= -\frac{1}{h^2} \int_{s_{2j}}^{s_{2j+2}} (s-s_{2j})(s-s_{2j+2})w(s)ds, \\
 v_{2j} &= \frac{1}{2h^2} \left\{ \int_{s_{2j-2}}^{s_{2j}} (s-s_{2j-2})(s-s_{2j-1})w(s)ds, \right. \\
 &\quad \left. + \int_{s_{2j}}^{s_{2j+2}} (s-s_{2j+1})(s-s_{2j+2})w(s)ds \right\}, \quad j \neq 0 \text{ or } m, \\
 v_n &= \frac{1}{2h^2} \int_{b-h}^b (s-s_{2m-2})(s-s_{2m-1})w(s)ds.
 \end{aligned} \tag{2.9.7}$$

If $f''(x) \in C[a, b]$, then the error in this rule is of the order $O(h^3)$. Note that the error may not be of the order $O(h^4)$ even if $f^{(4)}(x) \in C[a, b]$ unless $w(x) \equiv 1$ (see Wang 1976).

If the function $w(x)$ is of the form $(x-s)^{-\alpha}g(x, s)$, then the GENERALIZED TRAPEZOIDAL RULE is obtained by taking $\alpha = 1/2$, $s_j = a + jh$, as above, $g(x, s) = 1$, and $x = s_m$, $m = 0, 1, \dots, n$. Then

$$\int_a^b (s_m - s)^{-1/2} f(s) ds = \sum_{j=0}^{n-1} \left[v_{0,m}^{(j)} f(s_j) + v_{1,m}^{(j)} f(s_{j+1}) \right], \tag{2.9.8}$$

where

$$\begin{aligned}
 v_{0,m}^{(j)} &= \frac{1}{h} \int_{s_j}^{s_{j+1}} (s_{j+1} - s)(s_m - s)^{-1/2} ds, \\
 v_{1,m}^{(j)} &= \frac{1}{h} \int_{s_j}^{s_{j+1}} (s - s_j)(s_m - s)^{-1/2} ds.
 \end{aligned} \tag{2.9.9}$$

Alternatively, if we set

$$\psi_0(r) = \int_0^a (1-s)|r-s|^{-1/2} ds, \quad \psi_1(r) = \int_0^a s|r-s|^{-1/2} ds,$$

then

$$v_{0,m}^{(j)} = \sqrt{h} \psi_0(m-j), \quad v_{1,m}^{(j)} = \sqrt{h} \psi_1(m-j), \tag{2.9.10}$$

where

$$\begin{aligned}
 \psi_0(r) &= \psi_2(r) - \psi_1(r), \\
 \psi_1(r) &= \frac{2}{3} \left[\frac{(r-1)^2}{|r-1|^{1/2}} - \frac{r^2}{|r|^{1/2}} \right] + r\psi_2(r), \\
 \psi_2(r) &= 2 \left[\frac{r}{|r|^{1/2}} - \frac{r-1}{|r-1|^{1/2}} \right].
 \end{aligned}$$

Further, the quadrature rule for $w(s) = \ln |s_m - s|$ is given by

$$\int_a^b \ln |s_m - s| f(s) ds = \sum_{j=0}^{n-1} \left[\hat{v}_{0,m}^{(j)} f(s_j) + \hat{v}_{1,m}^{(j)} f(s_{j+1}) \right], \quad (2.9.11)$$

where by setting

$$\begin{aligned} \hat{\psi}_0(r) &= \int_0^a (1-s) \ln |r-s| ds, \\ \hat{\psi}_1(r) &= \int_0^a s \ln |r-s| ds, \end{aligned}$$

we have

$$\begin{aligned} \hat{v}_{0,m}^{(j)} &= \frac{1}{2} h \ln h + h \hat{\psi}_0(m-j), \\ \hat{v}_{1,m}^{(j)} &= \frac{1}{2} h \ln h + h \hat{\psi}_1(m-i); \end{aligned} \quad (2.9.12)$$

or, alternatively, $\hat{\psi}_0(r) = \hat{\psi}_2(r) - \hat{\psi}_1(r)$, where

$$\begin{aligned} \hat{\psi}_1(r) &= \frac{1}{2} \left\{ (r-1)^2 \ln |r-1| - r^2 \ln |r| + \frac{1}{4} [r^2 - (r-1)^2] \right\} + r \hat{\psi}_2(r), \\ \hat{\psi}_2(r) &= r \ln |r| = (r-1) \ln |r-1| - 1. \end{aligned}$$

A word of caution: While computing above formulas for $v_{0,m}^{(j)}$ and $\hat{v}_{1,m}^{(j)}$, to avoid cancellation error take the limit values as $r \rightarrow 0$ or $r \rightarrow 1$. Also, note the following GENERALIZATIONS OF THE MIDPOINT RULE for even n :

$$\int_a^b |s_m - s|^{-1/2} f(s) ds = \sum_{j=0}^{n/2-1} w_m^{2j+1} f(a + (2j+1)h) \quad (2.9.13)$$

and

$$\int_a^b \ln |s_m - s| f(s) ds = \sum_{j=0}^{n/2-1} \hat{w}_m^{2j+1} f(a + (2j+1)h), \quad (2.9.14)$$

where

$$\begin{aligned} w_m^{2j+1} &= v_{0,m}^{(2j)} + v_{1,m}^{(2j)} + v_{0,m}^{(2j+1)} + v_{1,m}^{(2j+1)}, \\ \hat{w}_m^{2j+1} &= \hat{v}_{0,m}^{(2j)} + \hat{v}_{1,m}^{(2j)} + \hat{v}_{0,m}^{(2j+1)} + \hat{v}_{1,m}^{(2j+1)}. \end{aligned}$$

Thus,

$$w_m^{(2j+1)} = 2\sqrt{h} \left[\frac{m-2j}{|m-2j|^{1/2}} - \frac{m-2j-2}{|m-2j-2|^{1/2}} \right],$$

whence by taking the limit values we get

$$w_{2j+2}^{(2j+1)} = w_{2j}^{(2j+1)} = 2\sqrt{2h}.$$

Lastly, the generalized rules can be extended to the case when $f(x)$ is the polynomial interpolant. For example, let $h = (b - a)/n$, and $n = Nm$, where N and m are integers; set $s_j = a + jh$, $j = 1, \dots, n$. For $s_{lm} \leq x \leq s_{lm+m}$ approximate $f(x)$ by the interpolant $P_{0,1,\dots,n}(x) \equiv P_{lm,lm+1,\dots,lm+m}(x)$ of degree m such that $P_{0,1,\dots,n}(x)$ agrees with $f(x)$ at the points $s_{lm}, s_{lm+1}, \dots, s_{lm+m}$. Then

$$\int_a^b w(s)f(s)ds = \sum_{l=0}^{N-1} \int_{s_{lm}}^{s_{lm+m}} w(s)P_{0,1,\dots,n}(s)ds = \sum_{j=0}^n v_j f(s_j), \quad (2.9.15)$$

where

$$v_j = \begin{cases} v_{lm+i} = \int_{s_{lm}}^{s_{lm+m}} \prod_{\substack{j=lm \\ j \neq lm+i}} \frac{s - s_j}{s_{lm+i} - s_j} w(s) ds & \text{if } j = lm + i, i \neq 0, \\ v_{lm} = \int_{s_{lm}}^{s_{lm+m}} \prod_{l=m+1}^{lm+m} \frac{s - s_j}{s_{lm} - s_j} w(s) ds \\ \quad + \int_{s_{lm-m}}^{s_{lm}} \prod_{l=m-m}^{lm-1} \frac{s - s_j}{s_{lm+i} - s_j} w(s) ds & \text{if } j = lm. \end{cases} \quad (2.9.16)$$

2.9.1. Application to Integral Equations. A MODIFICATION OF THE QUADRATURE METHOD in the case when the kernel $k(x, s)$ of an integral equation is badly behaved at $x = s$, i.e., when it is discontinuous or when one of its derivatives is discontinuous at $x = s$, consists of writing the integral equation as

$$\phi(x) - \lambda \phi(x) \int_a^b k(x, s) [\phi(s) - \phi(x)] ds = f(x),$$

and using a quadrature rule to obtain

$$\{1 - \lambda A(x)\} \tilde{\phi}(x) - \lambda \sum_{j=0}^n w_j k(x, s_j) \{\tilde{\phi}(s_j) - \tilde{\phi}(x)\} = f(x), \quad (2.9.17)$$

where $A(x) = \int_a^b k(x, s) ds$. If we use the notation

$$\Delta(x) = \sum_{j=0}^n w_j k(x, s_j) - A(x), \quad (2.9.18)$$

we obtain from (2.9.17)

$$\{1 + \lambda \Delta(x)\} \tilde{\phi}(x) - \lambda \sum_{j=0}^n w_j k(x, s_j) \tilde{\phi}(s_j) = f(x). \quad (2.9.19)$$

If we set $x = x_i, i = 0, 1, \dots, n$, in (2.9.19), we have the MODIFIED QUADRATURE RULE

$$\{1 + \lambda \Delta(x_i)\} \tilde{\phi}(x) - \lambda \sum_{j=0}^n w_j k(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad (2.9.20a)$$

which in matrix notation is

$$(\mathbf{I} + \lambda (\mathbf{\Delta} - \mathbf{KD})) \tilde{\Phi} = \mathbf{f}, \quad (2.9.20b)$$

where \mathbf{I} is the identity matrix, $\mathbf{k} = (k(x_i, s_j))_{ij}$, $\mathbf{\Delta} = \text{diag}\{\Delta(x_0), \Delta(x_1), \dots, \Delta(x_n)\}$, and $\mathbf{D} = \text{diag}\{w_0, w_1, \dots, w_n\}$. Note that the integral $A(x)$ needs to be computed accurately, either analytically or numerically, for this method.

2.10. Iterative and Adaptive Schemes

The production of automatic integration codes has been a favorite research topic since the 1960s. A number of *automatic integrators* have been developed to numerically integrate a function of one or more variables over a finite interval. Initially only functions of one variable were considered. These computer programs are said to be user-friendly, in the sense that the user enters the limits of integration, selects the routine for computation of $f(x)$, provides a tolerance ε , and enters the upper bound N for the number of functional computations. Then the program exits either (i) with the computed value I of the integral which is correct within the tolerance, which means that either $|I_a^b(f) - I| \leq \varepsilon$, or $\frac{|I_a^b(f) - I|}{I_a^b(|f|)} \leq \varepsilon$, or (ii) with a statement that the upper bound N was attained but the tolerance was not achieved, and the computed result may be the “best” value of the integral determined by the program. More sophisticated programs require, for example, that

$$|I_a^b(f) - I| \leq \max \left\{ \varepsilon_{\text{abs}}, \varepsilon_{\text{rel}} |I_a^b(f)| \right\},$$

where ε_{abs} and ε_{rel} are absolute and relative tolerances, respectively (Rice 1971).

Automatic integration falls into two classes (Shampine and Allen 1973, p. 67ff): iterative or noniterative, and adaptive or nonadaptive. The iterative schemes consist in computing successive approximations to the integral until an agreement with the prescribed tolerance is achieved, but in noniterative schemes the information from the first approximation is carried over to generate the second approximation, which then becomes the final result. In adaptive schemes the points at which the integration is carried out are chosen in a manner that is dependent on the nature of the integrand,

whereas in nonadaptive schemes the integration points are chosen in a fixed manner which is independent of the nature of the integrand, although the number of these points depends on the integrand.

An integration rule must not only approximate the value of an integral as closely as possible but also assess its error and try to produce a numerical value that satisfies certain accuracy criteria imposed by the user. Naturally more accurate results may take more computer time. In order to balance the computer time vis-a-vis accuracy, we need an iterative method that computes a sequence of approximate values with increasing accuracy and terminates with the best value when its accuracy requirement is satisfied.

2.10.1. An Iterative Method for Simpson's Rule. Consider Simpson's rule (2.5.6). Consider the first approximate value $I_a^b(f) \approx S_1(f)$. Now, partition the interval $[a, b]$ into several subintervals. Suppose, for example, in the case of bisection, i.e., a partition in half, we consider $I_a^b(f) \approx S_2(f)$. We can assume that the error in $S_2(f)$ is smaller than the difference $|S_2(f) - S_1(f)|$. To be more precise, let us assume that $f(x)$ is smooth. Then from (2.5.5) we have

$$I_a^b(f) = S_1(f) - \frac{|b-a|^5}{2880} f^{(4)}(\xi_1), \quad a < \xi_1 < b.$$

We apply this result to each half subinterval and get

$$\begin{aligned} I_a^b(f) &= \int_a^{(a+b)/2} f(x) dx + \int_{(a+b)/2}^b f(x) dx \\ &= S_2(f) - \frac{|b-a|^5}{2880} \frac{1}{2^5} [f^{(4)}(\xi_{21}) + f^{(4)}(\xi_{22})], \end{aligned}$$

where $a < \xi_{21} < \frac{a+b}{2} < \xi_{22} < b$. Let us further assume that the interval $[a, b]$ is small enough so that we can take $f^{(4)}(x)$ as a constant quantity denoted by $f^{(4)}$. Then

$$\begin{aligned} I_a^b(f) &\approx S_1(f) - \frac{|b-a|^5}{2880} f^{(4)}, \\ I_a^b(f) &\approx S_2(f) - \frac{|b-a|^5}{2880} f^{(4)} \frac{1}{2^4}, \end{aligned}$$

which gives

$$S_2(f) - S_1(f) \approx -\frac{2^4 - 1}{2^4} \frac{|b-a|^5}{2880} f^{(4)}.$$

Hence,

$$I_a^b(f) - S_2(f) \approx \frac{1}{15} [S_2(f) - S_1(f)]. \quad (2.10.1)$$

This relationship enables us to compute the error in the repeated Simpson's rule. Since the rule $S_n(f)$ applies to n equal subintervals $[a + (k-1)h, a + kh]$, $k = 0, 1, \dots, n$, of the given interval $[a, b]$, we apply the rule $S_{2n}(f)$, which amounts to the bisection of each of these subintervals and the application of the Simpson's rule to each part, and use formula (2.10.1) to estimate the error over each N subintervals. If we add all approximate integrals and the error terms, we get

$$I_a^b(f) - S_{2n}(f) \approx \frac{1}{15} [S_{2n}(f) - S_n(f)].$$

For example, let us compute an approximate integral $Q(f)$ such that $|I_a^b(f) - Q(f)| \leq \varepsilon$, where $\varepsilon > 0$ is a prescribed quantity, often known as the tolerance. We compute a sequence of approximations $S_{2^k}(f)$, $k = 0, 1, \dots$, and check the difference $|S_{2^{k+1}}(f) - S_{2^k}(f)|$. When this difference becomes less than ε , we stop and take $S_{2^{k+1}}(f)$ as $Q(f)$. In fact, we only compute the error to be less than $\varepsilon/15$. Or, we may compute the value of

$$Q(f) = S_{2^{k+1}}(f) + \frac{1}{15} |S_{2^{k+1}}(f) - S_{2^k}(f)|,$$

which removes the estimated error.

Remember that in this kind of iterative method the assumption that the quantity $f^{(4)}$ is taken as constant is important. Such an assumption is valid if $f^{(4)}$ is continuous and $N = 2^k$ is taken sufficiently large and ε is small. However, one must be quite suspicious if the above formula terminates while N is quite small. But then it may be the case because the problem was initially simple.

This method becomes inefficient in one respect. Since the interval $[a, b]$ is divided into many subintervals, and we compute two approximations $S_2(f)$ and $S_1(f)$ in each subinterval, we partition again if the agreement is not satisfactory. The agreement may be satisfactory in almost all subintervals, but we may encounter a large disagreement in one subinterval, which may affect all subintervals. This situation is remedied by adaptive processes which are described below.

2.10.2. An Adaptive Quadrature with Trapezoidal Rule. The quadrature rules generally assume that all integrands behave uniformly in the interval $[a, b]$. But most functions (integrands) vary more rapidly in one part of the interval $[a, b]$ than in another. As such the quadrature rules undergo certain disadvantages which can be corrected by using an adaptive quadrature formula. We will use the trapezoidal rule T_a^b to approximate the integral $I_a^b f$ in such a way that $|I_a^b f - T_a^b| \leq \varepsilon$, where ε is the specified tolerance. This is achieved by splitting the interval $[a, b]$ into a sequence of subintervals $[x_{i-1}, x_i]$ of length $h_i = x_i - x_{i-1}$, $i = 1, \dots, n$, with $x_0 = a$ and $x_n = b$. Then the total combined error from each subinterval is given by

$$E_T = -\frac{h_i^3}{12} f''(\xi_i), \quad x_{i-1} < \xi_i < x_i, \quad i = 1, \dots, n.$$

Note that the magnitude of this error depends on h_i and $f''(\xi_i)$; thus, in the case when $|f''(\xi_i)|$ is large, we need a smaller h_i to control the error. This means that we choose the sizes of the subintervals such that the contribution to the error from each subinterval is approximately the same. Let $I_{x_{i-1}}^{x_i}$ and $T_{x_{i-1}}^{x_i}$ denote the integral and its trapezoidal approximation in the subinterval $[x_{i-1}, x_i]$, respectively. If

$$|I_{x_{i-1}}^{x_i} - T_{x_{i-1}}^{x_i}| \leq \frac{h_i \varepsilon}{b-a},$$

then the total error will be less than ε . This process starts by obtaining the approximation by the trapezoidal rule on the entire interval $[a, b]$. Thus, we have

$$T_0^1 = \frac{b-a}{2} [f(a) + f(b)] = \frac{h_0}{2} [f(a) + f(b)], \quad \text{where } h_0 = b-a.$$

The next approximation T_0^2 is obtained by splitting the interval $[a, b]$ into two equal subintervals of size $h_i = h_0/2$, i.e.,

$$\begin{aligned} T_0^2 &= \frac{1}{2} \frac{h_0}{2} \left[f(a) + 2f\left(a + \frac{h_0}{2}\right) + f(b) \right] \\ &= \frac{1}{2} \left[T_0^1 + h_0 f\left(a + \frac{h_0}{2}\right) \right] \\ &= \frac{1}{2} T_0^1 + h_1 f(a + h_1) \quad \text{where } h_1 = \frac{h_0}{2}. \end{aligned}$$

The errors in these two approximations are

$$I - T_0^1 = -\frac{f''(\xi_1)}{12} h_0^3, \quad a < \xi_1 < b, \quad (2.10.2)$$

$$I - T_0^2 = -\frac{2f''(\xi_2)}{12} \left(\frac{h_0}{2}\right)^3, \quad a < \xi_2 < b. \quad (2.10.3)$$

The factor 2 appears in the error estimate (2.10.3) because of integration over two subintervals. Let us assume that $f''(x)$ is almost constant on the interval $[a, b]$, say, equal to $f''(\eta)$, then subtracting the above two error estimates we obtain

$$T_0^2 - T_0^1 = \frac{f''(\eta)}{12} \left(\frac{h_0}{2}\right)^3 (2 - 2^3),$$

which gives

$$\frac{f''(\eta)}{12} \left(\frac{h_0}{2}\right)^3 = -\frac{T_0^2 - T_0^1}{6}. \quad (2.10.4)$$

If we substitute (2.10.4) into the right side of (2.10.3), we obtain the error estimate

$$I - T_0^2 \approx \frac{1}{3} |T_0^2 - T_0^1|. \quad (2.10.5)$$

This shows that the error in the second approximation T_0^2 is approximately one-third of the difference $|T_0^2 - T_0^1|$, which can be easily computed. Thus, if the error

$$E_0 = \frac{1}{3} |T_0^2 - T_0^1| \leq \varepsilon, \quad (2.10.6)$$

then we accept T_0^2 as the required approximation of I_a^b . But if the condition (2.10.6) is not satisfied, then we first consider the left subinterval $[a, a + h_1]$ and then to the right subinterval $[a + h_1, b]$, and obtain the approximations to the integrals in those intervals, which satisfy a condition of the type (2.10.6) with tolerance $\varepsilon/2$ instead of ε . This process is repeated over the subinterval where the condition of the type (2.10.6) is not satisfied, until the approximations to the integral over each subinterval becomes accurate within the proper tolerance.

EXAMPLE 2.10.1. (Atkinson and Hatley, p. 238ff) Compute $\int_0^1 \frac{1}{1+x} dx$ using the above adaptive method. Note that the exact value is $\ln 2 = 0.6931$. We will take the tolerance as $\varepsilon = 0.005$. First, we compute T_0^1 over the entire interval $[0, 1]$:

$$T_0^1 = \frac{1}{2} \left(\frac{1}{1} + \frac{1}{2} \right) = \frac{3}{4} = 0.75.$$

We split the interval into two equal subintervals, and compute

$$T_0^2 = \frac{0.5}{2} \left[\frac{1}{1} + 2 \left(\frac{1}{1+0.5} \right) + \frac{1}{2} \right] = 0.7083,$$

$$\frac{1}{3} |T_0^2 - T_0^1| = 0.0139 \not\leq 0.005 = \varepsilon.$$

Thus, the tolerance is not satisfied in this interval size. So we consider the first subinterval $[0, 0.5]$. Here $h = 0.5$ and the error estimate is $\varepsilon/2 = 0.0025$. The first approximation on $[0, 0.5]$ is $T_0^1 = \frac{0.5}{2} \left(1 + \frac{2}{3} \right) = 0.4167$, and the second approximation is $T_0^2 = \frac{0.5}{4} \left[1 + 2 \left(\frac{4}{5} \right) + \frac{2}{3} \right] = 0.4083$. Then the error estimate is

$$\frac{1}{3} |T_0^2 - T_0^1| = \frac{1}{3} |0.0084| = 0.0028 \not\leq 0.0025.$$

Thus, the error estimate T_0^2 is not sufficiently accurate. Next, we split the interval $[0, 0.5]$ into two subintervals $[0, 0.25]$ and $[0.25, 0.5]$ and consider the integral in each, with tolerance $\varepsilon/4 = 0.00125$ in each. On the subinterval $[0, 0.25]$ we find that $T_0^1 = \frac{0.25}{2} \left(1 + \frac{4}{5} \right) = 0.225$, and $T_0^2 = \frac{0.25}{4} \left[1 + 2 \left(\frac{8}{9} \right) + \frac{4}{5} \right] = 0.2236$. The error estimate is

$$\frac{1}{3} |T_0^2 - T_0^1| = \frac{1}{3} (0.0014) = 0.0005 < 0.00125.$$

This is the first contribution to the integral over the entire interval, which we write as $\text{sum}_1 = 0.2236$. Next, we consider the right subinterval $[0.25, 0.5]$, in which $T_0^1 = \frac{0.25}{2} \left(\frac{4}{5} + \frac{2}{3} \right) = 0.1833$, and $T_0^2 = \frac{0.25}{4} \left[\frac{4}{5} + 2 \left(\frac{8}{11} \right) + \frac{2}{3} \right] = 0.1826$. The error estimate is

$$\frac{1}{3} |T_0^2 - T_0^1| = \frac{1}{3} (0.0007) = 0.0002 < 0.00125.$$

We write this contribution as $\text{sum}_2 = 0.1826$. Adding these two contributions we obtain $I_0^1(f) \approx \text{sum}_1 + \text{sum}_2 = 0.2236 + 0.1826 = 0.4062$. Next, we consider the right half interval $[0.5, 1]$, in which the tolerance is 0.0025. In this subinterval we have $T_0^1 = \frac{0.5}{2} \left(\frac{2}{3} + \frac{1}{2} \right) = 0.2917$, and $T_0^2 = \frac{0.5}{4} \left[\frac{2}{3} + 2 \left(\frac{4}{7} \right) + \frac{1}{2} \right] = 0.2887$. The error estimate is

$$\frac{1}{3} |T_0^2 - T_0^1| = \frac{1}{3} (0.003) = 0.001 < 0.00125.$$

We write this contribution as $\text{sum}_3 = 0.2887$. Adding this contribution to the previous sums, we find that $I_0^1(f) \approx 0.4062 + 0.2887 = 0.6949$. Since $|0.6931 - 0.6949| = 0.0018 < 0.005$, we stop the adaptive process. Thus, the approximate value of the integral is 0.6949. ■

The adaptive process can be based on any quadrature rule, and its accuracy is based on the number of points involved. Below we describe the adaptive process based on the Simpson's rule; this process is often used.

2.10.3. An Adaptive Method Based on Simpson's Rule. We will discuss the adaptive scheme for the Simpson's rule. Let $L = b - a$ denote the length of the interval $[a, b]$. First, we divide this interval into two equal parts, and compute

$$Q_1(f) = L \cdot \frac{1}{6} \cdot \left[f(a) + 4f\left(\frac{L}{2}\right) + f(b) \right],$$

and

$$Q_{11}(f) = \left(\frac{L}{2}\right) \cdot \frac{1}{6} \cdot \left[f(a) + 4f\left(a + \frac{L}{4}\right) + f\left(\frac{L}{2}\right) \right],$$

$$Q_{12}(f) = \left(\frac{L}{2}\right) \cdot \frac{1}{6} \cdot \left[f\left(a + \frac{L}{4}\right) + 4f\left(a + \frac{3L}{4}\right) + f(b) \right].$$

Then ask

Is $|Q_1 - (Q_{11} + Q_{12})| \leq \varepsilon$?

If the answer is 'yes', then $Q_{11} + Q_{12}$ is the result, i.e., $\int_a^b f(x) dx \approx Q_{11} + Q_{12}$.

If the answer is 'no', since $Q_{11} = \int_a^{a+L/2} f(x) dx$, we take the first half interval $[a, a + L/2]$, divide it into two equal parts, and compute

$$Q_{111}(f) = \left(\frac{L}{2^2}\right) \cdot \frac{1}{6} \cdot \left[f(a) + 4f\left(a + \frac{L}{8}\right) + f\left(a + \frac{L}{4}\right) \right],$$

$$Q_{112}(f) = \left(\frac{L}{2^2}\right) \cdot \frac{1}{6} \cdot \left[f\left(a + \frac{L}{4}\right) + 4f\left(a + \frac{3L}{8}\right) + f\left(a + \frac{L}{2}\right) \right].$$

Then ask

$$\boxed{\text{Is } |Q_{11} - (Q_{111} + Q_{112})| \leq \varepsilon/2?}$$

If ‘yes’, then $\int_a^{a+L/2} f(x) dx \approx Q_{111} + Q_{112}$. If ‘no’, repeat this process on the right half interval $[a + l/2, b]$, and compute

$$Q_{121}(f) = \left(\frac{L}{2^2}\right) \cdot \frac{1}{6} \cdot \left[f\left(a + \frac{L}{2}\right) + 4f\left(a + \frac{L}{8}\right) + f\left(a + \frac{3L}{4}\right) \right],$$

$$Q_{122}(f) = \left(\frac{L}{2^2}\right) \cdot \frac{1}{6} \cdot \left[f\left(a + \frac{3L}{4}\right) + 4f\left(a + \frac{7L}{8}\right) + f(b) \right].$$

Then ask

$$\boxed{\text{Is } |Q_{12} - (Q_{121} + Q_{122})| \leq \varepsilon/2?}$$

If ‘yes’, then $\int_{a+L/2}^b f(x) dx \approx Q_{121} + Q_{122}$. If ‘no’, repeat the third and fourth quarters of the interval $[a, b]$ by asking the question for each quarter, and continuing this process of bisecting the subinterval to the right until approximation is found for the whole interval.

The number of evaluations increase as we reach higher levels in this scheme. Therefore, there is a practical need to restrict the number of levels used. Once the maximum number of levels is reached, we can accept the last computed approximation and move to the right, or terminate the process in a predetermined manner. The accuracy of the values of $f(x)$ determines the accuracy of the value of the integral. As we approach higher levels, the lengths of the intervals as well as the magnitudes of the corresponding integrals over these intervals decrease, thus resulting in significant relative errors. At some point these errors become so large that further refinement becomes fatal. But the above adaptive scheme is refined (repeated) only for that subinterval where the result does not confirm to the tolerance criterion. This reduces the number of levels considerably, and thus this scheme enhances the accuracy of the Simpson’s rule.

The major difficulty in an adaptive process lies in the task of keeping track of the stage that has been reached; we should know which subinterval is processed and which subinterval is the next one to consider. If the derivatives of f change rapidly in some subinterval, we may be required to create a large number of nested subintervals before we attain the required accuracy. However, in computer codes there is no such difficulty because these codes allow recursion.

2.10.4. Convergence. Let ε denote the permissible error (tolerance) over each subinterval. Thus, if the integral $\int_a^b f(x) dx$ is computed with tolerance ε , then a natural choice for tolerance for each if the integrals $\int_a^{(a+b)/2} f(x) dx$ and $\int_{(a+b)/2}^b f(x) dx$ is $\varepsilon/2$. Thus, as we split further in an adaptive process, the error in

a subinterval $[\alpha, \beta] \subset [a, b]$ can be specified by

$$|I_\alpha^\beta(f) - Q_i(f)| \leq \left| \frac{\beta - \alpha}{b - a} \right| \varepsilon, \quad (2.10.7)$$

where $Q_i(f)$ denotes the quadrature rule used at the stage of this refinement in the subinterval $[\alpha, \beta]$. If the rule $Q_i(f, \alpha, \beta)$ is taken as the final approximate value of the integral, then

$$\begin{aligned} \left| I_a^b(f) - \sum_{[\alpha, \beta]} Q_i(f, \alpha, \beta) \right| &= \left| \sum_{[\alpha, \beta]} \left(I_\alpha^\beta(f) - Q_i(f, \alpha, \beta) \right) \right| \\ &\leq \sum_{[\alpha, \beta]} |I_\alpha^\beta(f) - Q_i(f, \alpha, \beta)| \leq \sum_{[\alpha, \beta]} \left| \frac{\beta - \alpha}{b - a} \right| \varepsilon = \varepsilon. \end{aligned}$$

This estimate suggests that the separate errors add up to the total allowable error. Some of the separate errors may be on the high side, but then the others are on the low side, so that their variations eventually cancel out. However, Shampine and Allen (1973, p. 72) have noted that “experience suggests that when splitting an interval in half, the error allowed be split by roughly $1/\sqrt{2}$ instead of $1/2$, for efficiency’s sake.”

The absolute error, defined by $|I_a^b(f) - Q(f)|$, is however not suitable for an adaptive code because it depends on the scaling of $f(x)$. Instead, we often use the relative error

$$\frac{|I_a^b(f) - Q(f)|}{|I_a^b(f)|}, \quad (2.10.8)$$

although it is found to be unsatisfactory in many cases. Let us consider the above adaptive process. Suppose in the first test we ask: Is $\frac{|(Q_{11} + Q_{12}) - Q_1|}{|(Q_{11} + Q_{12})|} \leq \varepsilon$?

This kind of test is found to be sensitive to computational errors. For example, if the values of the function $f(x)$ are large but the value of its integral is small, then we may have $Q_{11} \approx -Q_{12}$, so that the denominator may show severe cancellation and a case of overflow. Thus, the errors in Q_{11} and Q_{12} become more significant, and the above test in the adaptive process fails to be reliable.

Instead of the error (2.10.8), the relative L_1 -error test provided by

$$\frac{|I_a^b(f) - Q(f)|}{I_a^b(|f|)} \quad (2.10.9)$$

is free from the shortcomings of a relative test and can be used with advantage in adaptive codes, where the code computes $\int_a^b f(x) dx$ as well as $\int_a^b |f(x)| dx$. Note that if $f(x)$ is of one sign in the interval $[a, b]$, then the L_1 -error is the same as the relative error. But if $f(x)$ is of an oscillatory type, then $f(x)$ may not be small enough, but its integral may be. This error so computed will depend on the absolute

value which may not be small, and this may result in some difficult situations while using the L_1 -error test.

In order to integrate approximately a given function there are many cases where the direct integration may be unreasonable. In such cases we can use the following methods and transformations prior to the application of an adaptive computer code.

1. SPLIT THE INTERVAL OF INTEGRATION. If the function $f(x)$ is discontinuous at a point $c \in [a, b]$, we should split the problem of integrating $f(x)$ over the interval $[a, b]$ into two integrals $\int_a^c f(x) dx$ and $\int_c^b f(x) dx$ and use the code to compute each integral separately and then add the results. If $f'(x)$ is discontinuous at a point c , then we split the adaptive computer code at the point c .

EXAMPLE 2.10.2. Let

$$f(x) = \begin{cases} -1 & \text{if } 0 \leq x < 1/3, \\ 1 & \text{if } 1/3 \leq x \leq 1. \end{cases}$$

Then we compute $\int_0^{1/3} f(x) dx$ and $\int_{1/3}^1 f(x) dx$ separately, and add the two results. ■

2. CHANGE OF VARIABLES. Sometimes a change of variables is required or becomes desirable. For example, in the case of the improper integral

$$\int_a^\infty f(x) dx, \quad a > 0, \quad (2.10.10)$$

where the interval of integration is infinite, we set $x = 1/t$. This changes the integral (2.10.10) into $\int_0^{1/a} g(t) dt$, where $a > 0$, and $g(t) = \frac{f(1/t)}{t^2}$. Note that the point $x = \infty$ is mapped onto $t = 0$ and we have $\lim_{t \rightarrow 0} g(t) = \lim_{x \rightarrow \infty} x^2 f(x)$.

EXAMPLE 2.10.3. Consider the integral $\int_1^\infty \frac{e^{-x}}{x} dx$. Set $x = 1/t$. Then this integral is transformed into $\int_0^1 \frac{e^{-1/t}}{t} dt$. Here, $t = 0$ is an ordinary point for $g(t) = \frac{e^{-1/t}}{t}$, since $\lim_{t \rightarrow 0} g(t) = 0$. In the particular case when the lower limit of integration in (2.10.10) is 0 instead of $a > 0$, the above transformation does not work, but the transformation $t = e^{-x}$ does, and we get $\int_0^\infty f(x) dx = \int_0^1 \frac{f(-\ln t)}{t} dt = \int_0^1 h(t) dt$. ■

Another case of an improper integral occurs when the integrand becomes infinite at some interior point c of the interval $[a, b]$. In this case we first split the integral at the point c and integrate both parts separately. For example, consider the integrand $f(x) = \frac{g(x)}{(x-c)^\alpha}$, where $g(x)$ exists and is nonzero, and $0 < \alpha < 1$. We

set $x - c = t^\beta$, and choose β such that $\beta(1 - \alpha) \equiv n$ is a positive integer. Then

$$\int_c^b \frac{g(x)}{(x - c)^\alpha} dx = \beta \int_0^{(b-c)^{1/\beta}} g(c + t^\beta) t^{n-1} dt. \quad (2.10.11)$$

The integral (2.10.11) is continuous and finite if g is. A particular case is when $\alpha = m/k$, where m and k are integers. Then we set $\beta = k$ and $n = k - m \geq 1$, and the transformed integral is $\int_0^{(b-c)^{1/k}} g(c + t^k) t^{k-m-1} dt$, which is smooth if g is.

EXAMPLE 2.10.4. Consider

$$\int_0^1 \frac{e^x}{\sqrt{x}} dx. \quad (2.10.12)$$

By setting $x = t^2$ we transform this integral into

$$2 \int_0^1 e^{t^2} t dt, \quad (2.10.13)$$

which can be computed by using a computer code like SIMP with a tolerance of 10^{-5} , giving the result as 2.925301. The exact value is 2.92530349, which matches with the Mathematica result. ■

3. SUBTRACTING OUT SINGULARITIES. We write $f(x)$ as $f_1(x) + f_2(x)$, where $f_1(x)$ is relatively smooth and $f_2(x)$ contains the awkward part of $f(x)$ which can be integrated analytically. Then

$$\int_a^b f(x) dx = \int_a^b f_1(x) dx + \int_a^b f_2(x) dx, \quad (2.10.14)$$

and integrate the first integral numerically and the second analytically.

EXAMPLE 2.10.5. Consider $\int_0^1 \sin \sqrt{x} dx$. The integrand has an infinite derivative at $x = 0$. Since $\sin \sqrt{x} = \sqrt{x}$ for small values of x , we write

$$\int_0^1 \sin \sqrt{x} dx = \int_0^1 [\sin \sqrt{x} - \sqrt{x}] dx + \int_0^1 \sqrt{x} dx,$$

thus subtracting the ‘singularity’. The first integral is integrated numerically and the second analytically. Note that the integrand $\sin \sqrt{x} - \sqrt{x}$ in the first integral is differentiable at $x = 0$ since

$$\lim_{x \rightarrow 0} \frac{d}{dx} [\sin \sqrt{x} - \sqrt{x}] = \lim_{x \rightarrow 0} \frac{\cos \sqrt{x} - 1}{2\sqrt{x}} = 0.$$

For values close to $x = 0$ the quantity $\sin \sqrt{x} - \sqrt{x}$ loses significance as we subtract two almost equal quantities. But this is not important since the integrand tends to

zero as $x \rightarrow 0$. (The code **SIMP** applied directly to $f(x) = \sin \sqrt{x}$ with the tolerance 10^{-5} gives the result 0.6023364, with the estimated accuracy of 5×10^{-7} . The correct value of the integral is $2[\sin(1) - \cos(1)] = 0.6023374$. Hence, the true accuracy is 10^{-6} . The second integral in (2.10.14) computed analytically gives the result -0.06432933 with an estimated error of 2×10^{-8} . Adding these two we get the answer 0.6023373, with an estimated accuracy 3×10^{-8} and a true accuracy of 1.5×10^{-7} .) We note in passing that the change of variable $x = t^2$ transforms this integral to $\int_0^1 2t \sin t \, dt$, which gives the result as 0.6023364 by using the code **SIMP**, with an estimated accuracy of 5.2×10^{-7} and a true accuracy of 1.7×10^{-8} . ■

Another case to be considered is when $f(x)$ can be written as $f(x) = S(x)g(x)$, where $S(x)$ behaves badly at $c \in [a, b]$, and $g(x)$ has first n derivatives at c . In this case we write

$$f_2(x) = S(x) \left[g(c) + (x-c)g'(c) + \cdots + \frac{(x-c)^n}{n!} g^{(n)}(c) \right],$$

$$f_1(x) = f(x) - f_2(x).$$

Then we can analytically compute the integrals

$$\int_a^b f_2(x) \, dx = \sum_{k=0}^n \int_a^b S(x) \frac{(x-c)^k}{k!} g^{(k)}(c) \, dx,$$

and numerically compute the integral

$$\int_a^b f_1(x) \, dx = \int_a^b S(x) \left[g(x) - \sum_{k=0}^n \frac{g^{(k)}(c)}{k!} (x-c)^k \right] dx.$$

EXAMPLE 2.10.6. Consider the above example with $f(x) = \sin \sqrt{x}$, where we write $f(x) = \sqrt{x} \frac{\sin \sqrt{x}}{\sqrt{x}}$, and take $g(x) = \frac{\sin \sqrt{x}}{\sqrt{x}}$, $c = 0$, and $n = 0$. Then $f_2(x) = \sqrt{x}$, and $f_1(x) = \sin \sqrt{x} - \sqrt{x}$. This splitting is already treated in Example 2.10.5. If we take $n = 1$, then we have $f_2(x) = \sqrt{x} \left(1 - \frac{x}{6} \right)$, and $f_1(x) = \sin \sqrt{x} - f_2(x)$. Using the tolerance of 10^{-5} the integrand $f_1(x)$ gives the integral value as 0.002337339 (using **SIMP**) with the estimated error 1.1×10^{-7} . The final answer is found to be 0.6023374 with an estimated accuracy of 1.8×10^{-9} . ■

EXAMPLE 2.10.7. (Shampine and Allen 1973) Consider the model of a lightening rod in the form of an ellipsoidal column that projects above a flat plane in the (x, y) -plane with the rod along the z -axis. The potential function is defined by

$$V(x, y, z) = -z + Az \int_{\lambda}^{\infty} \frac{du}{\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)^3}}, \quad (2.10.15)$$

where A is a constant that depends on the shape of the rod and is given by

$$\frac{1}{A} = \int_0^\infty \frac{du}{\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)^3}},$$

and the value of λ is the smallest positive root of the equation

$$\frac{x^2}{a^2 + \lambda} + \frac{y^2}{b^2 + \lambda} + \frac{z^2}{c^2 + \lambda} - 1 = 0,$$

which is found to be 5928.359 (compare with the Mathematica value 5925.37, see [ex2.10.7.nb](#) on the CD-R). We will compute V at $x = 50 = y = z$ for $a = 1, b = 2, c = 100$, and $\lambda = 5928.359$. Note that the integrand $1/\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)^3}$ is well defined since it tends to zero as $u \rightarrow \infty$. Thus, we set $u = 1/t$, which changes the integral in (2.10.15) into

$$\int_0^{1/\lambda} \frac{dt}{t^2 \sqrt{(a^2 + 1/t)(b^2 + 1/t)(c^2 + 1/t)^3}}. \quad (2.10.16)$$

The expression (2.10.16) does not behave nicely for computation, so we rearrange it as

$$\int_0^{1/\lambda} \sqrt{\frac{t}{(a^2 t + 1)(b^2 t + 1)(c^2 t + 1)^3}} dt. \quad (2.10.17)$$

Shampine and Allen's code **SIMP** with a tolerance of 10^{-5} gives the value of this integral as 5.705946×10^{-7} with an estimated accuracy of 6.9×10^{-7} (compare with the Mathematica value 5.70592×10^{-7}). The integrand in (2.10.17) is nearly \sqrt{t} near $t = 0$, which gets difficult to integrate because its derivative becomes infinite near $t = 0$. Therefore, if we set $t = w^2 = 1/u$ in (2.10.17), the integral becomes

$$\int_0^{1/\lambda} \frac{2w^2}{\sqrt{(a^2 w^2 + 1)(b^2 w^2 + 1)(c^2 w^2 + 1)^3}} dw,$$

which is a bit easier to compute with **SIMP**, giving the value 5.705914×10^{-7} with an estimated accuracy of 1.8×10^{-7} (the Mathematica value for this integral is still the same as above 5.70592×10^{-7}). To compute the constant A we split the corresponding integral as

$$\int_0^\infty \frac{du}{\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)^3}} = \left(\int_0^\lambda + \int_\lambda^\infty \right) \frac{du}{\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)^3}},$$

which gives the value of $1/A = 7.788616 \times 10^{-6}$ (compare with the Mathematica value 7.78868×10^{-6}), thus $A = 1.283935 \times 10^5$ (compare with the Mathematica

value 1.28391×10^5 on the CD-R). Hence, $V = -46.337$, which compares very well with the Mathematica value -46.337 , (see [ex2.10.7.nb](#) on the CD-R). ■

2.11. Test Integrals

This section provides a list of test integrals which appear in Engels (1980). They are useful in testing various quadrature rules. The following notation is used: Let

$F_k(x) = \sum_{j=0}^{n-1} (-1)^j (j+1) x^{k-j-1}$; $G_k(x) = x^{-k}$; $\pi = 3.14159$; $s_m(x) = \tan \frac{\pi x}{2} \sin(m\pi x)$; $t_m(x) = \frac{\sin mx}{\sin \pi x}$; $u_{k,m}(x) = x^k \sin(m\pi x)$; and $v_{k,m}(x) = [mx] x^{k-1}$, where $[x]$ is the step function. The exact as well as approximate value of each integral is presented.

1. $\int_0^1 F_1(x) dx = 1$
2. $\int_0^1 F_2(x) dx = -3/2$
3. $\int_0^1 F_3(x) dx = 7/3$
4. $\int_0^1 F_4(x) dx = -35/12$
5. $\int_0^1 F_5(x) dx = 37/10$
6. $\int_0^1 F_6(x) dx = -259/60 \approx -4.316666666666667$
7. $\int_0^1 F_7(x) dx = 533/105 \approx 5.076190476190476$
8. $\int_0^1 F_8(x) dx = -1599/280 \approx -5.710714285714285$
9. $\int_0^1 F_9(x) dx = 1627/252 \approx 6.456349206349207$
10. $\int_0^1 F_{10}(x) dx = -17897/2520 \approx -7.101984126984127$
11. $\int_0^1 F_{11}(x) dx = 18107/2310 \approx 7.838528138528138$

12. $\int_0^1 F_{12}(x) dx = -235391/27720 \approx -8.49173881673882$
13. $\int_0^1 F_{13}(x) dx = 237371/25740 \approx 9.22187257187257$
14. $\int_0^1 F_{14}(x) dx = -1237371/24024 \approx -9.88057775557776$
15. $\int_0^1 F_{15}(x) dx = 95549/9009 \approx 10.6059496059496$
16. $\int_0^1 F_{16}(x) dx = -1624333/144144 \approx -11.26882145632146$
17. $\int_0^1 F_{17}(x) dx = 1632341/136136 \approx 11.99051683610507$
18. $\int_0^1 F_{18}(x) dx = -31014479/24504485 \approx -12.65665666033313$
19. $\int_0^1 F_{19}(x) dx = 155685007/11639628 \approx 13.37542806350856$
20. $\int_0^1 F_{20}(x) dx = -155685007/11085360 \approx -14.04419946668399$
21. $\int_0^1 (10x - 1)(10x - 1.1)(10x - 1.2)(10x - 1.3) dx = 1627279/1500$
 $\approx 1085.252666666667$
22. $\int_{0.01}^{1.1} G_3(x) dx = 5000 - 1/2.42 \approx 4999.586776859504$
23. $\int_{0.01}^{1.1} G_4(x) dx = (1.0(06) - 1/1.331)/3 \approx 333333.0828950663$
24. $\int_{0.01}^{1.1} G_5(x) dx = 2.5(07) - 1/5.8564 \approx 610.1808091361587$
25. $\int_0^1 (1+x)^{-1} dx = \ln 2 \approx 0.6931471805599453$
26. $\int_0^1 (1+x^2)^{-1} dx = \pi/4 \approx 0.7853981633974483$
27. $\int_0^1 (1+x^4)^{-1} dx = \left(\ln \frac{2+\sqrt{2}}{2-\sqrt{2}} + \pi \right) / \sqrt{32} \approx 0.866972987339911$
28. $\int_{-1}^1 (1+x^2+x^4)^{-1} dx = \frac{\ln 9}{4} + \frac{\pi}{\sqrt{12}} \approx 1.456205826451164$
29. $\int_{-1}^1 (1.005+x^2)^{-1} dx = \frac{2}{\sqrt{1.005}} \tan^{-1} \frac{1}{\sqrt{1.005}} \approx 1.56439644406905$

$$30. \int_0^{10} 50(2500x^2 + 1)/\pi \, dx = \tan^{-1} 500/\pi \approx 0.4993638028710166$$

$$31. \int_{-1}^1 (x^2 + 10^{-k})^{-1} \, dx = 2 \cdot 10^{k/2} \tan^{-1} (10^{k/2}), \quad k = 2(1)6$$

$$\approx \begin{cases} 29.42255348, & k = 2, \\ 97.3465489, & k = 3, \\ 312.159332, & k = 4, \\ 991.458833, & k = 5, \\ 3139.5926, & k = 6, \end{cases}$$

$$32. \int_0^1 (1 + 5x^2)^{-1} \, dx = \frac{\tan^{-1} \sqrt{5}}{\sqrt{5}} \approx 0.5144128009905458$$

$$33. \int_0^1 (1 + 10x^2)^{-1} \, dx = \frac{\tan^{-1} \sqrt{10}}{\sqrt{10}} \approx 0.3998760050557662$$

$$34. \int_0^1 (1 - 0.5x^2)^{-1} \, dx = \frac{1}{2\sqrt{0.5}} \ln \left(\frac{1 + \sqrt{0.5}}{1 - \sqrt{0.5}} \right) \\ \approx 1.246450480280461$$

$$35. \int_0^1 (1 - 0.98x^2)^{-1} \, dx = \frac{1}{2\sqrt{0.98}} \ln \left(\frac{1 + \sqrt{0.98}}{1 - \sqrt{0.98}} \right) \\ \approx 2.670965314886704$$

$$36. \int_0^1 (1 - 0.998x^2)^{-1} \, dx = \frac{1}{2\sqrt{0.998}} \ln \left(\frac{1 + \sqrt{0.998}}{1 - \sqrt{0.998}} \right) \\ \approx 3.803756514651015$$

$$37. \int_0^1 \frac{2^r}{1 + 2^r (x - \alpha)^2} \, dx \\ = \begin{cases} \pi & \text{if } r = 2, \alpha = 1/2, 1/3, \\ 2^{(r+2)/2} \tan^{-1} 2^{(r+2)/2} & \text{if } r > 2, \alpha = 1/2, 1/3, \\ 2^{r/2} [\tan^{-1} (\frac{2}{3} 2^{r/2}) + \tan^{-1} (\frac{1}{3} 2^{r/2})] & \text{if } r \geq 2, \alpha = 1/2, 1/3 \end{cases}$$

$$38. \int_0^1 x^{3/2} \, dx = 0.4$$

$$39. \int_0^1 x^{5/2} \, dx = 2/7$$

$$40. \int_0^1 \sqrt[k]{x} \, dx = 2^k / (1 + 2^k), \quad k = 1(1)4$$

$$\approx \begin{cases} 0.6666666666666666, & k = 1 \\ 0.8, & k = 2 \\ 0.8888888888888889, & k = 3 \\ 0.941176470588235, & k = 4 \end{cases}$$

41. $\int_0^1 \sqrt{|x^2 - 0.25|^k} dx \approx \begin{cases} 0.4647525054, & k = 1, \\ 0.1488716212, & k = 3, \\ 0.06551476837, & k = 5. \end{cases}$
42. $\int_{-9}^{100} |x|^{-1/2} dx = 26$
43. $\int_0^1 \sqrt[5]{x} dx = 5/6 \approx 0.8333333333333333$
44. $\int_0^1 \sqrt[10]{x} dx = 10/11 \approx 0.909090909090909$
45. $\int_{-1}^1 \sqrt{|x + 0.5|} dx = \sqrt{1.5} + \sqrt{0.5}/3 \approx 1.460447131787105$
46. $\int_0^1 |x - \beta|^\alpha dx = \frac{\beta^{\alpha+1} + (1 - \beta)^{\alpha+1}}{\alpha + 1};$
for $\alpha = 0.1(0.1)0.5$, $\beta = 0, \frac{1}{2}, \frac{1}{3}$
47. $\int_0^1 |x - \beta|^\alpha \ln |x - \beta| dx = \frac{\beta^{\alpha+1}}{(\alpha + 1)^2} [(\alpha + 1) \ln \beta - 1]$
 $+ \frac{(1 - \beta)^{\alpha+1}}{(\alpha + 1)^2} [(\alpha + 1) \ln(1 - \beta) - 1];$
for $\alpha = 0.1(0.1)0.5$, $\alpha = -0.55(-0.55) - 0.75$, $\beta = 0, \frac{1}{2}, \frac{1}{3}$
48. $\int_0^1 e^x dx = e - 1 \approx 1.718281828459045$
49. $\int_0^1 \frac{1}{e^x + 1} dx = \ln \frac{2e}{e + 1} \approx 0.3798854930417224$
50. $\int_0^1 \frac{x}{e^x + 1} dx \approx 0.1705573495024382$
51. $\int_0^{10} \sqrt{50} e^{-50\pi x^2} dx = \frac{1}{2} \sqrt{\pi/\dot{\pi}} \operatorname{erf}(50 s \sqrt{2\dot{\pi}})$
 $\approx 0.5000002111661001$
52. $\int_0^{10} 25 e^{-25x} dx = 1 - e^{-250} \approx 1$
53. $\int_0^1 (e^{-x} - e^{-10x}) dx = 0.9 + 0.1 e^{-10} - e^{-1}$
 $\approx 0.5321250988215339$
54. $\int_0^1 2 \left(e^{-9x^2} + e^{-1024(x-0.25)^2} \right) / \sqrt{\pi} dx = 1/16 + \operatorname{erf}(3)/3$
 $\approx 0.3958259698343338$
55. $\int_0^{10} \ln x dx = 10 \ln 10 \approx 14.02585092994046$

56. $\int_{10^{-4}}^7 \ln x \cdot \sin x \, dx = \ln 10^{-4} \cos 10^{-4} - \ln 7 \cos 7$
 $+ \text{Ci}(10^{-4}) - \text{Ci}(7) \approx -1.967546385989968$
57. $\int_0^1 (2^x x) / (2^x - 1) \, dx \approx 1.711857371268652$
58. $\int_0^1 \sin(\pi x) \, dx = 2/\pi \approx 0.6366197723675814$
59. $\int_0^1 \cos x \, dx = \sin 1 \approx 0.841470984807897$
60. $\int_0^1 2 / (2 + \sin(10\pi x)) \, dx = 2/\sqrt{3} \approx 1.154700538379252$
61. $\int_0^{2\pi} x \sin(30x) \cos x \, dx = -60\pi/899 \approx -0.2096724796611653$
62. $\int_0^{2\pi} x \sin(30x) \cos(50x) \, dx = 3\pi/80 \approx 0.1178097245096172$
63. $\int_0^{2\pi} (\pi x \sin(30x)) / \sqrt{4\pi^2 - x^2} \, dx = \pi^3 J_1(60\pi)$
 $\approx -1.271629809446774$
64. $\int_{-1}^1 (0.92 \cosh x - \cos x) \, dx = 0.92(e - 1/e) - 2 \sin 1$
 $\approx 0.4794282266888015$
65. $\int_0^1 \sin(100\pi x) \, dx = 0$
66. $\int_{1/20}^{1/3} (1/x) \sin(1/x) \, dx = \text{Si}(20) - \text{Si}(3) \approx -0.3004108269560286$
67. $\int_0^1 s_1(x) \, dx = 1$
68. $\int_0^1 s_2(x) \, dx = -1$
69. $\int_0^1 s_3(x) \, dx = 1$
70. $\int_0^1 s_4(x) \, dx = -1$
71. $\int_0^1 t_2(x) \, dx = 0$
72. $\int_0^1 t_3(x) \, dx = 1$

$$73. \int_0^1 t_4(x) dx = 0$$

$$74. \int_0^1 u_{0,m}(x) dx = 2/(m\pi), \quad m = 5, 15, 25$$

$$\approx \begin{cases} 0.1273239544735163, & m = 5 \\ 0.04244131815783875, & m = 15 \\ 0.02546479089470326, & m = 25 \end{cases}$$

$$75. \int_0^1 u_{0,m}(x) dx = 0, \quad m = 10, 20$$

$$76. \int_0^1 u_{1,m}(x) dx = 1/(m\pi), \quad m = 5, 15, 25$$

$$77. \int_0^1 u_{1,m}(x) dx = -1/(m\pi), \quad m = 10, 20$$

$$\approx \begin{cases} -0.03183098861837907, & m = 10 \\ -0.01591549430918954, & m = 20 \end{cases}$$

$$78. \int_0^1 u_{2,m}(x) dx = 1/(m\pi) - 4/(m\pi)^3, \quad m = 5, 15, 25$$

$$\approx \begin{cases} 0.06262992813489575, & m = 5 \\ 0.02118243503810966, & m = 15 \\ 0.01272413905453673, & m = 25 \end{cases}$$

$$79. \int_0^1 u_{2,m}(x) dx = -1/(m\pi), \quad m = 10, 20$$

$$\approx \begin{cases} -0.03183098861837907, & m = 10 \\ -0.01591549430918954, & m = 20 \end{cases}$$

$$80. \int_0^1 u_{3,m}(x) dx = 1/(m\pi) - 6/(m\pi)^3, \quad m = 5, 15, 25$$

$$\approx \begin{cases} 0.06211390358396455, & m = 5 \\ 0.0211633230177048, & m = 15 \\ 0.01272001085812928, & m = 25 \end{cases}$$

$$81. \int_0^1 u_{3,m}(x) dx = 6/(m\pi)^3 - 1/(m\pi), \quad m = 10, 20$$

$$\approx \begin{cases} -0.03163747941177987, & m = 10 \\ -0.01589130565836463, & m = 20 \end{cases}$$

$$82. \int_0^1 (\operatorname{sech}^2(10x - 2) + \operatorname{sech}^4(100x - 40) + \operatorname{sech}^6(1000x - 600)) dx$$

$$= (\tanh 8 + \tanh 2)/10 + 2/150 + 2/1875$$

$$\approx 0.2108027549615858$$

83. $\int_0^1 v_{0,m}(x) dx = \sum_{n=1}^{m-1} n \ln \left(\frac{n+1}{n} \right), \quad m = 5(5)25$
84. $\int_0^1 v_{1,m}(x) dx = \frac{m-1}{2}, \quad m = 5(5)25$
85. $\int_0^1 v_{2,m}(x) dx = \frac{4m^2 - 3m - 1}{12m}, \quad m = 5(5)25$
86. $\int_0^1 (x+k) dx = 1.5 \quad \text{for } k/3 \leq x \leq (k+1)/3, k = 0(1)2$
87. $\int_0^1 \begin{cases} 0, & 0.49 < x < 0.5, \\ 1000 (x - x^2), & \text{otherwise} \end{cases} dx$
 $= 1000 (0.49^2/2 - 0.49^3/3 + 1/12) \approx 164.167$
88. $\int_0^1 \begin{cases} 1/(x+2), & 0 \leq x \leq e-2, \\ 0, & e-2 \leq x \leq 1 \end{cases} dx = 1 - \ln 2$
 $\approx 0.3068528194400547$
89. $\int_0^1 \begin{cases} 0, & 0 \leq x < 0.3, \\ 1, & 0.3 \leq x \leq 1 \end{cases} dx = 0.7$
90. $\int_0^1 \begin{cases} 0, & x = 0, \\ 1, & 0 < x \leq 1 \end{cases} dx = 2$
91. $\int_0^1 \begin{cases} 1, & x = 0, \\ x/(e^x - 1), & 0 < x \leq 1 \end{cases} dx \approx 0.777504635$
92. $\int_0^1 \begin{cases} 100, & x = 0, \\ \sin(100\dot{\pi}x)/x, & 0 < x \leq 1 \end{cases} dx = (\text{Si}(100\dot{\pi}) - \text{Si}(10\dot{\pi})) / \dot{\pi}$
 $\approx 0.00909864525656933$
93. $\int_0^1 \begin{cases} 50, & x = 0, \\ \frac{\sin^2(50\dot{\pi}x)}{50(\dot{\pi}x)^2}, & 0 < x \leq 1 \end{cases} dx = \frac{\text{Si}(100\dot{\pi})}{\dot{\pi}} + \frac{\cos(100\dot{\pi}) - 1}{100(\dot{\pi})^2}$
 $\approx 0.498987230169528$
94. $\int_0^1 \begin{cases} 0, & 0 \leq x \leq 10^{-15}, \\ \ln x, & 10^{-15} \leq x \leq 1 \end{cases} dx = 10^{-15} - 1 + 15 \cdot 10^{-15} \ln 10$
 $\approx -0.999999999999965$
95. $\int_{-1}^2 \begin{cases} e^x, & -1 \leq x < 0, \\ e^{1-x}, & 0 \leq x \leq 2 \end{cases} dx = 1 + e - 2/e \approx 2.98252294611616$
96. $\int_{-1}^{1.5} \begin{cases} e^{10x}, & -1 \leq x < 0.5, \\ e^{10(1-x)}, & 0.5 \leq x \leq 1.5 \end{cases} dx = (2e^5 + e^{-5} - e^{-10}) / 10$
 $\approx 29.68330107522225$

3

Gaussian Quadrature

The interpolatory quadrature rules are based on the notion that the nodes (quadrature points) must be preassigned equidistantly or with some other kind of fixed distribution. As mentioned in Kowalewski (1932), Gauss was the first to realize that a suitable variation of the nodes leads to better accuracy in general, and this fundamental result of Gauss started many variations and generalizations of the Gaussian formulas of the type $I_a^b(f) = \sum_{k=0}^n w_k f(x_k)$, where the weights w_k are positive zeros of certain orthogonal polynomials and the nodes x_k are distinct points in the interval $(-1, 1)$. We will study some extended Gaussian rules and provide tables of their nodes and weights. Gaussian moments are discussed in detail and presented in a tabular form. The optimal Gaussian rule of the highest degree of precision is presented.

3.1. Gaussian Rules

Let $\{\phi_n(x)\}$ denote a sequence of polynomials, where $\phi_n(x) \in \mathcal{P}_n$. These polynomials are orthogonal with respect to a weight function $w(x)$ over the interval $[a, b]$. We can write $\phi_n(x) = a_n p_n(x)$, where $a_n \neq 0$ is the coefficient of x^n in $\phi_n(x)$, and $p_n(x)$ is an orthogonal polynomial. Then, we have

$$\int_a^b w(x) \phi_i(x) \phi_j(x) dx = 0 \quad \text{for } i \neq j. \quad (3.1.1)$$

The *Christoffel-Darboux identity* is

$$\sum_{k=0}^n \frac{\phi_k(x) \phi_k(y)}{\gamma_k} = \frac{\phi_{n+1}(x) \phi_n(y) - \phi_n(x) \phi_{n+1}(y)}{\alpha_n \gamma_n (x - y)}, \quad (3.1.2)$$

where

$$\alpha_n = \frac{a_{k+1}}{a_k}, \quad \gamma_n = \int_a^b w(x) \phi_k^2(x) dx. \quad (3.1.3)$$

Now, set $y = x_i$, where x_i are the zeros of $\phi_n(x)$. Then we get

$$\sum_{k=0}^{n-1} \frac{\phi_k(x) \phi_k(x_i)}{\gamma_k} = -\frac{\phi_n(x) \phi_{n+1}(x_i)}{a_n \gamma_n (x - x_i)}. \quad (3.1.4)$$

Now, we multiply both sides of (3.1.4) by $w(x)\phi_0(x)$ and integrate over $[a, b]$. Then using (3.1.1) we get

$$\phi_0(x_i) = -\frac{\phi_{n+1}(x_i)}{\alpha_n \gamma_n} \int_a^b w(x) \frac{\phi_0(x) \phi_n(x)}{x - x_i} dx. \quad (3.1.5)$$

Since from the definition of the Lagrangian interpolation polynomial we have

$$l_i(x) = \frac{\pi_n(x)}{(x - x_i) \pi'_n(x_i)} = \frac{\phi_n(x)}{(x - x_i) \phi'_n(x_i)}, \quad (3.1.6)$$

and since $\phi_0(x) = \text{const}$, we find from (3.1.5) and (3.1.6) that

$$\begin{aligned} 1 &= -\frac{\phi_{n+1}(x_i)}{\alpha_n \gamma_n} \int_a^b w(x) \frac{\phi_n(x)}{x - x_i} dx \\ &= -\frac{\phi_{n+1}(x_i) \phi'_n(x_i)}{\alpha_n \gamma_n} \int_a^b w(x) l_i(x) dx \\ &= -\frac{\phi_{n+1}(x_i) \phi'_n(x_i)}{\alpha_n \gamma_n} w_i, \end{aligned} \quad (3.1.7)$$

where

$$w_i = -\frac{a_{n+1} \gamma_n}{a_n \phi_{n+1}(x_i) \phi'_n(x_i)} \quad \text{for } i = 1, \dots, n. \quad (3.1.8)$$

The error is given by

$$E_n = \frac{\gamma_n}{a_n^2 (2n)!} f^{(2n)}(\xi), \quad a < \xi < b. \quad (3.1.9)$$

Note that for the Legendre polynomials $P_n(x)$ these formulas give

$$\begin{aligned} \gamma_n &= \int_{-1}^1 P_n^2(x) dx = \frac{2}{2n+1}, \\ a_n &= \frac{(2n)!}{2^n (n!)^2}, \\ w_i &= -\frac{2}{(n+1) P_{n+1}(x_i) P'_n(x_i)}, \\ E_n &= \frac{2^{2n+1} (n!)^4}{(2n+1) [(2n)!]^3} f^{(2n)}(\xi), \quad -1 < \xi < 1. \end{aligned} \quad (3.1.10)$$

We consider quadrature rules of the form

$$I_a^b(f) \equiv \int_a^b f(x) dx = \sum_{i=0}^n w_i f(x_i), \quad (3.1.11)$$

where the nodes (abscissae) x_i are not equally spaced. If we replace f by an interpolating polynomial $p_n(x)$ constructed at the points x_i , $i = 0, 1, \dots, n$, then this polynomial has the Lagrangian form

$$p_n(x) = l_0(x)f(x_0) + \dots + l_n(x)f(x_n), \quad (3.1.12)$$

where $l_i(x)$, $i = 0, 1, \dots, n$, are defined by (1.4.3). If we integrate (3.1.12) over $a \leq x \leq b$, we obtain the right side of (3.1.11), where the weights w_i are given by

$$w_i = \int_a^b l_i(x) dx, \quad 0 \leq i \leq n, \quad (3.1.13)$$

Note that for equally-spaced nodes x_i this procedure leads to a different method of deriving the Newton-Cotes quadrature formulas. The error term (1.4.5) on integration over the interval $[a, b]$ gives

$$I_a^b f - \sum_{i=0}^n w_i f(x_i) = \frac{1}{(n+1)!} \int_a^b \pi_{n+1}(x) f^{(n+1)}(\xi) dx, \quad (3.1.14)$$

where $\pi_{n+1}(x) = (x - x_0)(x - x_1) \dots (x - x_n)$. Thus, the quadrature rule (3.1.11) is exact if $f \in \mathcal{P}_n$ because since $f^{(n+1)}(x) \equiv 0$ the right side of (3.1.14) vanishes. The rule (3.1.11) is exact for any linear combination of functions f and g if it is exact for the functions f and g separately. Thus, if α and β are any arbitrary real numbers, we have

$$\int_a^b (\alpha f(x) + \beta g(x)) dx = I_a^b f + I_a^b g = \sum_{i=0}^n w_i [\alpha f(x_i) + \beta g(x_i)].$$

This shows that the rule (3.1.11) is exact for $f \in \mathcal{P}_n$ if it is exact for the monomials $1, x, x^2, \dots, x^n$. In fact, the rule (3.1.11) is exact for x^j if

$$\int_a^b x^j dx = \sum_{i=0}^n w_i x_i^j. \quad (3.1.15)$$

Since the left side of (3.1.15) is known, we take $j = 0, 1, \dots, 2n+1$ and obtain a system of $(2n+2)$ equations to solve $2n+2$ unknowns w_i and x_i for $i = 0, 1, \dots, n$. If this system has a solution, the resulting quadrature rule will be exact for $f \in \mathcal{P}_{2n+1}$. In fact, $p_j(x)p_k(x) \in \mathcal{P}_{2n+1}$ for $j, k < n$, so that

$$\sum_{i=0}^n w_i p_j(x_i) p_k(x_i) = \int_a^b w(x) p_j(x) p_k(x) dx = \delta_{jk}.$$

Thus,

$$\langle f, g \rangle = \sum_{i=0}^n w_i f(x_i) g(x_i).$$

We will develop the error (3.1.14) in terms of the divided differences. Since

$$f(x) - p_n(x) = \pi_{n+1}(x) f[x, x_0, \dots, x_n],$$

we have

$$I_a^b f - \sum_{i=0}^n w_i f(x_i) = \int_a^b \pi_{n+1}(x) f[x, x_0, \dots, x_n] dx. \quad (3.1.16)$$

If $f[x, x_0, \dots, x_n] \in \mathcal{P}_m$, $m > 0$, then $f[x, x_0, \dots, x_{k+1}] \in \mathcal{P}_{m-1}$. This result follows from (1.3.7) which gives

$$f[x, x_0, \dots, x_{k+1}] = \frac{f[x_0, \dots, x_{k+1}] - f[x, x_0, \dots, x_k]}{x_{k+1} - x},$$

and since the numerator on the right side is a polynomial of degree m and has $(x - x_{k+1})$ as one of the factors, then $f \in \mathcal{P}_{m-1}$. Hence, if $f \in \mathcal{P}_{2n+1}$, we can show by induction that $f[x, x_0, \dots, x_n] \in \mathcal{P}_n$. Now, let $\{p_0, p_1, \dots, p_{n+1}\}$ be a set of orthogonal polynomials on $[a, b]$, and let $p_r \in \mathcal{P}_r$, $r = 0, 1, \dots, n+1$. Then for some set of real numbers $\alpha_0, \alpha_1, \dots, \alpha_n$, we have $f[x, x_0, \dots, x_n] = \alpha_0 p_0(x) + \alpha_1 p_1(x) + \dots + \alpha_n p_n(x)$. Then, because of the orthogonality relations

$$\int_a^b p_r(x) p_s(x) dx \begin{cases} = 0 & \text{for } r \neq s, \\ \neq 0 & \text{for } r = s, \end{cases}$$

the right side of (3.1.16) is zero if $\pi_{n+1}(x) = \alpha p_{n+1}(x)$ for some real $\alpha \neq 0$.

The Gaussian quadrature rules cannot in general be used for functions that are defined only at discrete points since such rules require that the functions be evaluated at specific points ξ_i which are the zeros of the related polynomials. However, in some experimental cases where there is complete freedom of choosing the data of functional values at the specific nodes ξ_i , the corresponding Gaussian rules can be used to evaluate $I_a^b(f)$. The error bounds are virtually impossible to obtain in such cases. But if the data is mostly error free, then a very high order interpolating polynomial may be effectively used to obtain a significantly accurate result. There is no practical advantage in using a Gaussian quadrature if the data is noisy and some smoothing is needed prior to the application of a specific Gaussian quadrature rule.

It must be noted that the Gaussian rules of all orders are also Riemann sums. These rules integrate exactly polynomials of any degree by a formula of the form (3.1.11).

3.2. Extended Gaussian Rules

The extended (repeated or compound) Gaussian rules are similar to the repeated trapezoidal, midpoint and Simpson's rules. If $f \in C^{2n+2}[-1, 1]$, the $(n + 1)$ -point Gaussian rule is of the form (3.1.11), where the error is given by

$$E_{n+1} = \frac{2^{2n+3} (n!)^4}{(2n+3) [(2n)!]^3} f^{(2n+2)}(\xi), \quad \xi \in (-1, 1). \quad (3.2.1)$$

This error decreases rapidly as n increases.

THEOREM 3.2.1. If $p_{2n+1}(x) \in \mathcal{P}_{2n+1}$, then the formula

$$\int_a^b w(x) p_{2n+1}(x) dx = \sum_{i=0}^n \alpha_i p_{2n+1}(x_i)$$

is exact if the points $x_i, i = 0, 1, \dots, n$, are the zeros of the orthogonal polynomial $\phi_{n+1}(x)$, and α_i are defined by

$$\alpha_i = \int_a^b w(x) l_i(x) dx.$$

PROOF. The polynomial $p_{2n+1}(x)$ can be written in the form

$$p_{2n+1}(x) = q(x) \phi_{n+1}(x) + r(x),$$

where $q(x)$ and $r(x)$ are polynomials of degree at most n . Since x_i are the zeros of $\phi_{n+1}(x)$, we get $p_{2n+1}(x_i) = r(x_i)$ for $i = 0, 1, \dots, n$. Also, since the quadrature rule

$$I_a^b(f) = \int_a^b w(x) f(x) dx = \int_a^b w(x) p_n(x) dx = \sum_{i=0}^n \alpha_i f_i = I_n(f)$$

is precise for n , we have

$$\int_a^b w(x) r(x) dx = \sum_{i=0}^n \alpha_i r(x_i).$$

Now, consider

$$\begin{aligned} I_a^b(p_{2n+1}) &= \int_a^b w(x) p_{2n+1}(x) dx = \int_a^b w(x) [q(x) \phi_{n+1}(x) + r(x)] dx \\ &= \int_a^b w(x) q(x) \phi_{n+1}(x) dx + \int_a^b w(x) r(x) dx. \end{aligned}$$

We can replace $q(x)$ by its unique representation in terms of the orthogonal polynomials $\phi_i(x)$, $i = 0, 1, \dots, n$; i.e., $q(x) = \sum_{i=0}^n c_i \phi_i(x)$. Then the first term on the right side in $I_{p_{2n+1}}$ becomes automatically zero because of the orthogonality relations of $\phi_i(x)$. Thus,

$$I_a^b(p_{2n+1}) = \int_a^b w(x) r(x) dx = \sum_{i=0}^n \alpha_i r(x_i) = \sum_{i=0}^n \alpha_i p_{2n+1}(x_i) = I_n p_{2n+1},$$

where $\alpha_i > 0$ denotes the weights. ■

THEOREM 3.2.2. (Johnson and Riess 1977, p. 326) The Gaussian quadrature formula has precision $2n + 1$ only if the points x_i , $i = 0, 1, \dots, n$, are the zeros of $\phi_{n+1}(x)$.

THEOREM 3.2.3. Let $f(x) \in C^{2n+2}[a, b]$. Then the error in using the Gaussian quadrature is given by

$$I_a^b(f) - I_n(f) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b w(x) T_{n+1}^2(x) dx,$$

where $T_n(x)$ is the Chebyshev polynomial of the first kind.

3.2.1. Gauss-Jacobi Rule. The Jacobi polynomials $P_n^{(\alpha, \beta)}(x)$ are the orthogonal polynomials with the weight function $w(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha > -1$, $\beta > -1$. The Gauss-Jacobi rule (also known as the Mehler quadrature formula) is defined by

$$\int_{-1}^1 (1-x)^\alpha(1+x)^\beta f(x) dx = \sum_{i=1}^n w_i f(x_i) + E, \quad (3.2.2)$$

where

$$w_i = -\frac{2n + \alpha + \beta + 2}{n + \alpha + \beta + 1} \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)}{(n + 1)! \Gamma(n + \alpha + \beta + 1)} \times \frac{2^{\alpha+\beta}}{P_n^{(\alpha, \beta)}(x) P_{n+1}^{(\alpha, \beta)}(x)}. \quad (3.2.3)$$

and the error term E_n in the n -point rule is

$$E_n = \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)\Gamma(n + \alpha + \beta + 1)}{(2n + \alpha + \beta + 1) [\Gamma(2n + \alpha + \beta + 1)]^2} \times \frac{n! 2^{2n + \alpha + \beta + 1}}{(2n)!} f^{(2n)}(\xi), \quad \xi \in (-1, 1). \quad (3.2.4)$$

The Gauss-Legendre rule is a special case of formula (3.2.3) with $\alpha = \beta = 0$. The Gauss-Chebyshev rule is another special case with $\alpha = \beta = -1/2$.

For integrands with the Jacobi weight function $w(x) = (1 - x)^\alpha(1 + x)^\beta$ Piessens and Branders (1973) use the formulas

$$\int_{-1}^1 (1 - x)^\alpha(1 + x)^\beta g(x) \, dx \approx \sum_{k=0}^N b_k G_k(\alpha, \beta) + E_N^1, \tag{3.2.5}$$

$$\int_{-1}^1 (1 - x)^\alpha(1 + x)^\beta \ln\left(\frac{1 + x}{2}\right) g(x) \, dx \approx \sum_{k=0}^N b_k I_k(\alpha, \beta) + E_N^2, \tag{3.2.6}$$

where $g(x)$ is assumed to have a rapidly convergent Chebyshev series expansion

$$g(x) = \sum_{k=0}^\infty a_k T_k(x),$$

and

$$\begin{aligned} b_k &= \frac{2}{N} \sum_{m=0}^{N''} g(x_m) T_k(x_m), \quad x_m = \cos \frac{m\pi}{N}, \\ G_n(\alpha, \beta) &= 2^{\alpha+\beta+1} \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} {}_3F_2\left[\begin{matrix} n, -n, \alpha+1 \\ \frac{1}{2}, \alpha+\beta+2 \end{matrix}; 1\right], \\ E_k^1 &\approx a_{k+1} (G_{k+1}(\alpha, \beta) - G_{k-1}(\alpha, \beta)), \\ E_k^2 &\approx a_{k+1} (I_{k+1}(\alpha, \beta) - I_{k-1}(\alpha, \beta)), \end{aligned}$$

and $I_n(\alpha, \beta)$ are obtained from the recurrence relation

$$\begin{aligned} (\alpha + \beta + n + 2) I_{n+1}(\alpha, \beta) + 2(\alpha - \beta) I_n(\alpha, \beta) + (\alpha + \beta - n + 2) I_{n-1}(\alpha, \beta) \\ = 2G_n(\alpha, \beta) - G_{n-1}(\alpha, \beta) - G_{n+1}(\alpha, \beta). \end{aligned}$$

EXAMPLE 3.2.1. Compute $\int_{-1}^1 (1 - x)^{1/2}(1 + x)^{1/2} g_i(x) \, dx$, $i = 1, 2$, where $g_1(x) = e^{-2x}$, and $g_2(x) = (x + 1.01)^{-3/2}$. The results are given in Table 3.2.1 (Piessens and Branders 1973).

Table 3.2.1. Exact Values and Absolute Errors.

	Exact	N	Gauss-Jacobi	Formula (3.2.5)-(3.2.6)
$g_1(x)$	2.1643953820	5	7.9(−7)	1.8(−6)
		6	6.0(−9)	7.2(−8)
$g_2(x)$	4.2785147337	10	2.7(−1)	2.5(−1)
		20	2.3(−2)	2.6(−1)
		50	8.1(−6)	9.3(−6)
		100	< 5.0(−11)	< 5.0(−11)

The value of these two integrals are $\frac{\pi}{2} I_1(2) \approx 2.4985665285$ and 5.7963478953 , respectively (by Mathematica), which casts doubt about the accuracy of the above method.

3.2.2. Gauss-Legendre Rule. This rule is a special case of the Gauss-Jacobi formula (3.2.3) with $\alpha = \beta = 0$. The weight function $w(x) = 1$ and the orthogonal polynomials $\phi_i(x)$ are the Legendre polynomials $P_i(x)$, $i = 1, \dots$, with $P_i(1) = 1$. This rule on the interval $[-1, 1]$ is given by (3.1.11), where the nodes x_i are the i -th zeros of $P_n(x)$; the weights are given by $w_i = \frac{2}{(1 - x_i^2) [P'_n(x_i)]^2}$; and the remainder is

$$R_n = \frac{2^{2n+1} (n!)^4}{(2n+1) [(2n)!]^3} f^{(2n)}(\xi), \quad -1 < \xi < 1.$$

The Gauss-Legendre rule for arbitrary interval $[a, b]$ is

$$\int_a^b f(y) dy = \frac{b-a}{2} \sum_{i=1}^n w_i f(y_i) + R_n,$$

where the nodes are $y_i = \left(\frac{b-a}{2}\right)x_i + \left(\frac{b+a}{2}\right)$; the related nodes x_i and the weights w_i are defined above; and

$$R_n = \frac{(b-a)^{2n+1} 2^{2n+1} (n!)^4}{(2n+1) [(2n)!]^3} f^{(2n)}(\xi), \quad a < \xi < b.$$

The rules (3.1.11) are exact for $f \in \mathcal{P}_{2n+1}$.

Using the first few Legendre polynomials $P_0(x) = 1$, $P_1 = x$, $P_2 = (3x^2 - 1)/2$, $P_3 = (5x^3 - 3x)/2$, we get

For $n = 0$ in (3.1.11) we have the Gauss-Legendre rule with one node at $x = 0$ which is the zero of $P_1(x)$: $I_{-1}^1 f = 2f(0)$, which is exact for $f \in \mathcal{P}_1$. This is comparable to the midpoint rule.

For $n = 1$ in (3.1.11) we have the Gauss-Legendre rule with two nodes at $x = \pm 1/\sqrt{3}$ which are the zeros of $P_2(x)$: $I_{-1}^1 f = f(-1/\sqrt{3}) + f(1/\sqrt{3})$, which is exact for $f \in \mathcal{P}_3$. This is comparable to the Simpson's rule.

For $n = 2$ in (3.1.11) we have the Gauss-Legendre rule with three nodes at $x = 0, \pm\sqrt{3/5}$ which are the zeros of $P_3(x)$: $I_{-1}^1 f = [5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})]/9$, which is exact for $f \in \mathcal{P}_5$.

The weights and nodes of the Gauss-Legendre rules for small $n = 1(1)5$ are as follows:

$$\begin{aligned}
 n = 1 : \quad & x_1 = 0, \quad w_1 = 2; \\
 n = 2 : \quad & x_1 = -x_2 = 1/\sqrt{3}, \quad w_1 = w_2 = 1; \\
 n = 3 : \quad & x_1 = -x_3 = \sqrt{3/5}, \quad x_2 = 0, \quad w_1 = w_3 = 5/9, w_2 = 8/9; \\
 n = 4 : \quad & x_{1,2} = -x_{4,3} = [(3 \pm \sqrt{4.8})/7]^{1/2}, \quad w_{1,2} = w_{4,3} = (1 \mp \sqrt{5/54})/2; \\
 n = 5 : \quad & x_{1,2} = -x_{5,4} = (5 \pm \sqrt{40/7})^{1/2}/3, \quad x_3 = 0, \\
 & w_{1,2} = w_{5,4} = (3.22 \mp 1.3 \sqrt{0.7})/9, \quad w_3 = 64/225.
 \end{aligned}$$

The following two properties are obvious: (i) $\sum_{i=0}^n w_i = 2$; and (ii) this rule is symmetric with respect to the point $\xi = 0$, i.e., if (ξ_i, w_i) belongs to the rule, so does $(-\xi_i, w_i)$.

For larger values of n the nodes and the weights are given in Table A.6 for $n = 2(1)10, 12, 16$. The files `gausspts4-6.nb`, `gausspts12.nb`, `gausspts13.nb`, `GaussLegendre.m` and `GaussLegendre.nb` on the CD-R are useful. Since this data is part of computational codes, these values are either incorporated in the codes or are generated to any degree required by the program incorporated in the codes. The Gauss-Legendre rules are mostly used in computer subroutines, because they have the highest possible degree of precision. The weights and nodes are generally floating point numbers. But the closed form of the nodes and weights for this quadrature for small $n = 1(1)5$ is very suitable for applications on electronic pocket computers where there is no storage for long floating point numbers. These nodes and weights are given below.

For the Gauss-Legendre rule, an interval $[a, b]$ can be transformed into $[-1, 1]$ by using the linear transformation

$$a = \frac{b+a}{2} + \frac{b-a}{2} \xi. \quad (3.2.7)$$

Then the Gauss-Legendre quadrature rule becomes

$$If = \frac{b-a}{2} \sum_{k=1}^n w_k f(\xi_k). \quad (3.2.8)$$

where the nodes x_k are the n zeros of the n -th degree Legendre polynomials.

EXAMPLE 3.2.2. (Hornbeck 1975, p. 156) Evaluate $\int_0^{\pi/2} x^2 \cos x \, dx$ by using the Gauss-Legendre quadrature with $n = 4$. The following table of nodes and weights for $n = 4$ will be used.

ξ_k	w_k
± 0.3399810436	0.6521451549
± 0.8611363116	0.3478548451

Since $x_i = \frac{\pi}{4} (1 + \xi_i)$, we get

$$\begin{aligned}x_1 &= \frac{\pi}{4} (1 - 0.8611363116) = 0.109063286, \\x_2 &= \frac{\pi}{4} (1 - 0.3399810436) = 0.518377676, \\x_3 &= \frac{\pi}{4} (1 + 0.3399810436) = 1.05241865, \\x_4 &= \frac{\pi}{4} (1 + 0.8611363116) = 1.46173304,\end{aligned}$$

which gives

$$\begin{aligned}f(x_1) &= x_1^2 \cos x_1 = 0.011824127, & f(x_2) &= x_2^2 \cos x_2 = 0.233412695, \\f(x_3) &= x_3^2 \cos x_3 = 0.548776921, & f(x_4) &= x_4^2 \cos x_4 = 0.232569839.\end{aligned}$$

Thus,

$$\begin{aligned}I &= \frac{b-a}{2} \sum_{i=1}^n w_i f(x_i) \\&= \frac{\pi}{4} [w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) + w_4 f(x_4)] \\&= \frac{\pi}{4} [(0.3478548451)(0.011824127) + (0.6521451549)(0.233412695) \\&\quad + (0.6521451549)(0.548776921) + (0.3478548451)(0.232569839)] \\&= 0.467402.\end{aligned}$$

This result is compared with the trapezoidal rule ($n = 3$), Simpson's rule ($n = 4$), and the exact solutions in Table 3.2.2. It is found that the Gauss-Legendre result is remarkably accurate with only 4 nodes. Note that both Gauss-Legendre and the trapezoidal rules involve 4 evaluations of $f(x)$ whereas the Simpson's rule requires 5 evaluations. ■

Table 3.2.2.

Gauss-Legendre	Trapezoidal ($n = 3$)	Simpson's ($4 = 4$)	Exact
0.467402	0.411411	0.46689	0.467401

EXAMPLE 3.2.3. (Ralston-Rabinowitz 1978, p. 117.) Compute $\int_1^3 \frac{dx}{x}$ with $n = 1$ and $h = 1$. We have

$$\begin{aligned}\int_1^3 \frac{dx}{x} &\approx \frac{1}{2} \sum_{i=0}^1 \left\{ \left[1 + \frac{1}{2} \left[\left(1 + \frac{1}{\sqrt{3}} \right) + 2i \right]^{-1} + \left[1 + \frac{1}{2} \left[\left(1 - \frac{1}{\sqrt{3}} \right) + 2i \right]^{-1} \right] \right\} \\&= 1.097713.\end{aligned}$$

The error is bounded by $0.000046 \approx \frac{1}{90} \frac{1}{(3)^5} < E_2 < \frac{1}{90} \approx 0.011111$. ■

3.2.3. Gauss-Laguerre Rule. A Gaussian quadrature over the interval $[0, \infty)$ with weight function $w(x) = e^{-x}$ (Abramowitz and Stegun 1968, p. 890). The abscissae for quadrature order n are given by the roots of the Laguerre polynomials $L_n(x)$. The weights are

$$w_i = -\frac{A_{n+1} \gamma_n}{A_n L'_n(x_i) L_{n+1}(x_i)} = \frac{A_n}{A_{n-1}} \frac{\gamma_{n-1}}{L_{n-1}(x_i) L'_n(x_i)},$$

where A_n is the coefficient of x^n in $L_n(x)$, given by $A_n = \frac{(-1)^n}{n!}$. Thus, $\frac{A_{n+1}}{A_n} = -\frac{1}{n+1}$, and $\frac{A_n}{A_{n-1}} = -\frac{1}{n}$. Also, $\gamma_n = \int_0^\infty w(x) [L_n(x)]^2 dx = 1$, which gives

$$\begin{aligned} w_i &= \frac{1}{(n+1) L'_n(x_i) L_{n+1}(x_i)} = -\frac{1}{n L_{n-1}(x_i) L'_n(x_i)} \\ &= \frac{1}{x_i [L'_n(x_i)]^2} = \frac{x_i}{(n+1)^2 [L_{n+1}(x_i)]^2}. \end{aligned}$$

The error term is given by

$$E_n = \frac{(n!)^2}{(2n)!} f^{(2n)}(\xi).$$

The nodes and weights for the Gauss-Laguerre rule are given in [Table A.7](#) for $n = 2, 4, 8, 10$. For $n = 2$ they have the exact values

$$\begin{aligned} n = 2 : \quad x_i &= 2 - \sqrt{2}, & w_i &= (2 + \sqrt{2})/4, \\ &= 2 + \sqrt{2}, & &= (2 - \sqrt{2})/4. \end{aligned}$$

3.2.4. Gauss-Hermite Rule. This is a Gaussian quadrature over the interval $(-\infty, \infty)$ (Abramowitz and Stegun 1968, p. 890). The nodes for quadrature of order n are given by the roots x_i of the Hermite polynomials $H_n(x)$, which occur symmetrically about 0. The weights are

$$w_i = -\frac{A_{n+1} \gamma_n}{A_n H'_n(x_i) H_{n+1}(x_i)} = \frac{A_n}{A_{n-1}} \frac{\gamma_{n-1}}{H_{n-1}(x_i) H'_n(x_i)},$$

where A_n is the coefficient of x^n in $H_n(x)$. For Hermite polynomials, $A_n = 2^n$, so $\frac{A_{n+1}}{A_n} = 2$. Additionally, $\gamma_n = \sqrt{\pi} 2^n n!$, so (see [Abramowitz and Stegun 1968, p. 890](#))

$$\begin{aligned} w_i &= -\frac{2^{n+1} n! \sqrt{\pi}}{H_{n+1}(x_i) H'_n(x_i)} = \frac{2^n (n-1)! \sqrt{\pi}}{H_{n-1}(x_i) H'_n(x_i)} \\ &= \frac{2^{n+1} n! \sqrt{\pi}}{[H'_n(x_i)]^2} = \frac{2^{n+1} n! \sqrt{\pi}}{[H_{n+1}(x_i)]^2} = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 [H_{n-1}(x_i)]^2}, \end{aligned}$$

where the following recurrence relation is used: $H'_n(x) = 2n H_{n-1}(x) = 2x H_n(x) - H_{n+1}(x)$. The error term is

$$E_n = \frac{n! \sqrt{\pi}}{2^n (2n)!} f^{(2n)}(\xi).$$

The nodes and weights can be computed analytically for small n as:

$$\begin{aligned} n = 2 : \quad & x_i = \pm 1/\sqrt{2}, & w_i &= \frac{1}{2} \sqrt{\pi}, \\ n = 3 : \quad & x_i = 0, & w_i &= \frac{2}{3} \sqrt{\pi}, \\ & x_i = \pm \frac{1}{2} \sqrt{6}, & w_i &= \sqrt{\pi}/6, \\ n = 4 : \quad & x_i = \pm \sqrt{\frac{3 - \sqrt{6}}{2}}, & w_i &= \frac{\sqrt{\pi}}{4(3 - \sqrt{6})}, \\ & x_i = \pm \sqrt{\frac{3 + \sqrt{6}}{2}}, & w_i &= \frac{\sqrt{\pi}}{4(3 + \sqrt{6})}. \end{aligned}$$

The nodes and the weights for the Gauss-Hermite rule are given in [Table A.8](#) for $n = 2, 4, 8, 16$.

3.2.5. Gauss-Radau Rule. A Gaussian quadrature-like formula for numerical estimation of integrals. It requires $m + 1$ points and fits all polynomials to degree $2m$, so it effectively fits exactly all polynomials of degree $2m - 1$. It uses a weight function $w(x) = 1$ in which the endpoint -1 in the interval $[-1, 1]$ is included in a total of n abscissae, giving $r - n - 1$ free abscissae. The general formula is

$$\int_{-1}^1 f(x) dx = \frac{2}{n^2} f(-1) + \sum_{i=2}^n w_i f(x_i).$$

The free nodes for $i = 2, \dots, n$ are the roots of the polynomial $\frac{P_{n-1}(x) + P_n(x)}{1 + x}$, where $P_n(x)$ is a Legendre polynomial. The weights of the free nodes are

$$w_i = \frac{1 - x_i}{n^2 [P_{n-1}(x_i)]^2} = \frac{1}{(1 - x_i) [P'_{n-1}(x_i)]^2}.$$

The error term is given by

$$E_n = \frac{2^{2n-1} n [(n-1)!]^4}{[(2n-1)!]^3} f^{(2n-1)}(\xi), \quad -1 < \xi < 1.$$

The nodes and weights are given in [Table A.9](#) for $n = 3(1)10$; for smaller values of n their exact values are

$$\begin{aligned} n = 2 : \quad x_i &= -1, & w_i &= \frac{1}{2}, \\ &= \frac{1}{3}, & &= \frac{3}{2}, \\ n = 3 : \quad x_i &= -1, & w_i &= \frac{2}{9}, \\ &= \frac{1}{5} (1 - \sqrt{6}), & &= \frac{1}{18} (16 + \sqrt{6}), \\ &= \frac{1}{5} (1 + \sqrt{6}), & &= \frac{1}{18} (16 - \sqrt{6}). \end{aligned}$$

For nodes and weights, see [radou.nb](#) on the CD-R.

3.2.6. Gauss-Lobatto Rule. When the Gaussian formula (3.1.11) is used with the polynomials $P'_{n-1}(x)$, where $P_n(x)$ are the Legendre polynomials, we get Lobatto's rule:

$$\int_{-1}^1 f(x) dx = \frac{2}{n(n-1)} [f(1) + f(-1)] + \sum_{i=1}^{n-1} w_i f(x_i) + R_n,$$

where the quadrature point x_i is the $(i-1)$ -st zero of $P'_{n-1}(x)$; this formula is exact if $f \in \mathcal{P}_{2n-1}$, and the weights $w_i = \frac{2}{n(n-1)[P_{n-1}(x_i)]^2}$ for $x_i \neq \pm 1$; and

$$R_n = \frac{-n(n-1)^3 2^{2n-1} [(2n-1)!]^4}{(2n-1)[(2n-2)!]^3} f^{(2n-2)}(\xi), \quad -1 < \xi < 1.$$

The 3-point Lobatto rule is Simpson's rule. The nodes and weights are given in [Table A.10](#) for $n = 3(1)10$. For nodes and weights, see [lobatto.nb](#) on the CD-R.

3.2.7. Gauss-Chebyshev Rule. In the quadrature rule

$$\int_a^b w(x) f(x) dx = \sum_{i=0}^n w_i f(x_i), \quad (3.2.9)$$

the weight w_i and the nodes x_i can be found for different orthogonal polynomials approximations of $f(x)$ such that formula (3.2.9) is exact for all $f \in \mathcal{P}_{2n+1}$. Thus, in particular, if $[a, b]$ is taken as $[-1, 1]$ and $w(x) = (1-x^2)^{-1/2}$, the orthogonal polynomials are the Chebyshev polynomials $T_N(x)$ of the first kind, and the resulting formulas are known as the Gauss-Chebyshev rule. Thus, by taking the interpolating polynomials as

$$p_n(x) = \sum_{i=0}^n l_i(x) f(x_i),$$

where x_i are the zeros of $T_n(x)$. Then, in view of (3.2.3) the weights w_i are given by

$$w_i = -\frac{\pi}{T_{n+1}(x_i)T'_n(x_i)}. \quad (3.2.10)$$

Putting $x = \cos \theta$, we have $T_n(x) = \cos n\theta$, and $T'_n(x) = \frac{n \sin n\theta}{\sin \theta}$. Now we write $x_i = \cos \theta_i$. Then

$$\begin{aligned} T_{n+1}(x_i) &= \cos(n+1)\theta_i = \cos n\theta_i \cos \theta_i - \sin n\theta_i \sin \theta_i \\ &= \mp \sqrt{1 - x_i^2}, \quad \text{since } \cos n\theta_i = 0, \\ T'_n(x_i) &= \frac{n \sin n\theta_i}{\sin \theta_i} = \frac{\pm n}{\sqrt{1 - x_i^2}}, \end{aligned}$$

which gives

$$w_i = \frac{\pi}{n}. \quad (3.2.11)$$

This shows that for all Chebyshev rules the weights are all equal. The error in the n -point rule is given by

$$E_n = \frac{2\pi}{2^{2n}(2n)!} f^{(2n)}(\xi), \quad -1 < \xi < 1. \quad (3.2.12)$$

We choose $[a, b] = [-1, 1]$, $w(x) = (1 - x^2)^{-1/2}$, and the polynomials $q_i(x)$ as the normalized Chebyshev polynomials

$$q_i(x) = \begin{cases} \sqrt{\frac{2}{\pi}} T_i(x) & \text{for } i = 1, 2, \dots, n-1, \\ \sqrt{\frac{1}{\pi}} T_0(x) & \text{for } i = 0. \end{cases} \quad (3.2.13)$$

The nodes ξ_i for the n -point quadrature are the zeros of $T_n(x)$, defined by

$$\xi_i = \cos\left(\frac{(2i-1)\pi}{2n}\right), \quad i = 1, 2, \dots, n. \quad (3.2.14)$$

The rule with ξ_i given by (3.2.14) and the weight (3.2.10) is of degree $2n-1$, and is known as the *open Gauss-Chebyshev rule*, since the endpoints are not included as the nodes. The word ‘open’ is generally omitted since all Gaussian rules with positive weight function are of the open type. This rule is also known as Fejér’s first integration formula

$$\int_{-1}^1 f(x) dx = \sum_{i=1}^n w_i f\left(\cos \frac{(2i-1)\pi}{2n}\right), \quad f \in \mathcal{P}_{n-1}, \quad (3.2.15)$$

where the weights w_i are given by

$$w_i = \frac{2}{\pi} \left[1 - 2 \sum_{k=1}^{[n/2]} \frac{\cos(2k\theta_k)}{4k^2 - 1} \right]. \quad (3.2.16)$$

The (open) Gauss-Chebyshev rule is related to the midpoint rule with $w(x) = 1$, which is defined by

$$I_a^b f \approx h \sum_{i=1}^n f\left(a + \frac{(2i-1)h}{2}\right), \quad h = \frac{b-a}{2}.$$

This is easily seen by setting $[a, b] = [0, \pi]$ and $x = \cos \theta$; then the above midpoint rule changes to

$$\int_{-1}^1 \frac{f(\cos^{-1} x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n} \sum_{i=1}^n f\left(\frac{(2i-1)\pi}{2n}\right).$$

We can, however, construct the ‘closed’ Gauss-Chebyshev rule by including the endpoints $\xi_0 = 1$ and $\xi_n = -1$ as additional nodes. Then we get a rule with nodes $\xi_i = \cos(i\pi/n)$, $i = 0, 1, \dots, n$, and weights $w_i = \pi/n$ for $i = 1, 2, \dots, N$, and $w_0 = w_n = \pi/(2n)$. Thus, the ‘closed’ Gauss-Chebyshev rule is

$$\int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n} \sum_{j=0}^n f\left(\cos \frac{j\pi}{n}\right). \quad (3.2.17)$$

This rule can be obtained from the repeated trapezoidal rule by the same method as used in showing the relationship of the open Gauss-Chebyshev rule to the midpoint rule, although the relation does not clarify why the rule is of high degree. In practice we do not generally use the closed rule because sometimes it is not possible to include the endpoint nodes. However, the closed rule has the advantage in a situation where we carry out a sequence of computations by successively doubling n , because in the closed rule the n points ξ_i are the subset of the $2n$ points ξ_i , and the previous function evaluations can be used again.

EXAMPLE 3.2.4. (Delves and Mohamed 1974, p. 33) Compute $\int_{-1}^1 \frac{x^2 dx}{\sqrt{1-x^2}}$ by using both open and closed Gauss-Chebyshev rules, for $n = 2$. Note that $f(x) = x^2$. Then

- (i) *Open Gauss-Chebyshev rule:* For $n = 2$, $T_2(x) = 2x^2 - 1$, and its zeros are $\xi_1 = -1/\sqrt{2}$ and $\xi_2 = 1/\sqrt{2}$. The integral is exactly equal to $\frac{\pi}{2} \left[\left(-\frac{1}{\sqrt{2}} \right) + \left(\frac{1}{\sqrt{2}} \right) \right] = \frac{\pi}{2}$.

- (ii) *Closed Gauss-Chebyshev rule:* For $n = 2$ the nodes are $\xi_i = \cos \frac{i\pi}{2}$, $i = 0, 1, 2$, i.e., $\xi_0 = 1$, $\xi_1 = 0$, and $\xi_2 = -1$. The integral has the exact value $\frac{\pi}{2} \left[\frac{1}{2}(1)^2 + (0)^2 + \frac{1}{2}(-1)^2 \right] = \frac{\pi}{2}$. ■

EXAMPLE 3.2.5. (Ralston-Rabinowitz 1978, p. 110) Compute $If = \int_{-1}^1 \frac{e^x dx}{\sqrt{1-x^2}}$ correct to six decimal digits. Using (3.2.12) we find that the error for the n -point rule is bounded by

$$|E_n| \leq \frac{2ne}{2^{2n} (2n)!}.$$

Thus, $|E_4| \leq 1.66 \times 10^{-6}$, and $|E_5| \leq 4.6 \times 10^{-9}$. Hence, we apply the Gauss-Chebyshev rule for $n = 5$, which gives

$$If \approx \frac{\pi}{5} \sum_{i=1}^5 \exp \left| \cos \frac{(2i-1)\pi}{10} \right| = 3.977463. \blacksquare$$

If instead of the Chebyshev polynomial of the first kind $T_n(x)$ we take the interpolating polynomial as the Chebyshev polynomial of the second kind $U_n(x)$, we use the relation $U_n(\cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta}$ and obtain the quadrature rule

$$\int_{-1}^1 f(x) dx \approx \sum_{k=1}^n w_k f\left(\cos \frac{k\pi}{n+1}\right), \quad (3.2.18)$$

which is precise for $f \in \mathcal{P}_{n-1}$, where

$$w_k = \frac{2}{n+1} \left[1 - 2 \sum_{m=1}^{[(n-1)/2]} \frac{\cos(2m\theta_k)}{4m^2 - 1} - \frac{1}{p} \cos(p+1)\theta_k \right], \quad \theta_k = \frac{k\pi}{n+1}, \quad (3.2.19)$$

where $p = 2 \left\lfloor \frac{n+1}{2} \right\rfloor - 1$ is the largest odd integer $\leq n$. An alternative form of w_k is

$$w_k = \frac{4 \sin \theta_k}{n+1} \sum_{m=1}^{[(n-1)/2]} \frac{\sin(2m-1)\theta_k}{2m-1}. \quad (3.2.20)$$

As in the previous case, these weights can be proved to be positive. In either case, as $n \rightarrow \infty$, the Gauss-Chebyshev rules converge to $\int_{-1}^1 f(x) dx$ for all f , which are Riemann-integrable in $[-1, 1]$.

The equal-weight Chebyshev rule is

$$\int_{-1}^1 f(x) dx = \frac{2}{n} \sum_{i=1}^n f(x_i) + R_n,$$

where the node x_i is the i -th zero of the polynomial part of

$$x^n \exp \left\{ - \left(\frac{n}{2 \cdot 3 x^2} + \frac{n}{4 \cdot 5 x^3} + \frac{n}{6 \cdot 7 x^4} + \cdots \right) \right\},$$

which are given in [Table A.11](#) for $n = 2(1)9$; for $n = 8$ and $n \geq 10$ some of the values of x_i are complex; the remainder R_n is given by

$$R_n = \int_{-1}^1 \frac{x^{n+1}}{(n+1)!} f^{(n+1)}(\xi) dx - \frac{2}{n(n+1)!} \sum_{i=1}^n x_i^{n+1} f^{(n+1)}(\xi_i),$$

for $0 \leq \xi \leq x$ and $0 \leq \xi_i \leq x_i, i = 1, \dots, n$.

There are two Gauss-Chebyshev Rules on an arbitrary interval $[a, b]$:

1. Using the Chebyshev polynomials of the first kind, $T_n(x)$, where $T_n(1) = 1/2^{n-1}$, we have

$$\int_a^b \frac{f(y)}{\sqrt{(y-a)(b-y)}} dy = \sum_{i=1}^n w_i f(y_i) + R_n,$$

where the nodes $y_i = \frac{b+a}{2} + \frac{b-a}{2} x_i$, with $x_i = \cos \frac{(2i-1)\pi}{2n}$; the weights are the same as above.

2. Using the Chebyshev polynomials of the second kind

$$U_n(x) = \frac{\sin[(n+1) \arccos x]}{\sin(\arccos x)},$$

we get

$$\int_a^b f(y) \sqrt{(y-a)(y-b)} dy = \left(\frac{b-a}{2} \right)^2 \sum_{i=1}^n w_i f(y_i) + R_n,$$

where the nodes are y_i and the weights are the same as in 1 above.

3.2.8. Gauss-Log Rule. The Gaussian rule with a logarithmic singularity is

$$\int_0^1 \ln x f(x) dx = \sum_{i=1}^n w_i f(x_i) + R_n,$$

where $R_n = \frac{f^{(2n)}(\xi)}{(2n)!} r_n$, and the nodes and the weights are given in [Table A.12](#) for $n = 2, 4, 8, 16$.

3.3. Other Extended Rules

Some useful extended rules are as follows.

3.3.1. Clenshaw-Curtis Rules. It is well known that for smooth integrands $f(x)$ the Gaussian rules give better accuracy than the Newton-Cotes rules including the trapezoidal and Simpson's rules. Even if $f(x)$ is not smooth, the Gaussian rules provide results no worse than the other types of rules. From a practical point of view, the weight function $w(x) = 1$ is more common than the Chebyshev weight function $w(x) = 1/\sqrt{1-x^2}$. Often we write

$$I_{-1}^1(f) \equiv \int_{-1}^1 f(x) dx = \int_{-1}^1 \frac{g(x) dx}{\sqrt{1-x^2}}, \quad (3.3.1)$$

where $g(x) = \sqrt{1-x^2} f(x)$. But if $f(x)$ is smooth near $x = \pm 1$, $g(x)$ is not, and the Gauss-Chebyshev rule will provide the result which converges very slowly as N increases. However, the Clenshaw-Curtis rule (Clenshaw 1957, Clenshaw and Curtis 1960) removes this situation and provides an effective quadrature rule (see [Clenshaw and Curtis 1960](#)). Quadrature formulas based on Chebyshev nodes transformed to the interval of integration $[a, b]$ and known as the Clenshaw-Curtis formulas are more suitable for numerical integration than the Newton-Cotes formulas. The Clenshaw-Curtis formulas with the weight function $w(x) = 1$ are called modified Clenshaw-Curtis formulas. Consider the integral $I_{-1}^1(f)$ and assume that the integrand $f(x)$ is continuous and of bounded variation on $[-1, 1]$. Then $f(x)$ is approximated in terms of the Chebyshev polynomials of the first kind by

$$f(x) = \sum_{k=0}^n {}'' w_k T_k(x). \quad (3.3.2)$$

To determine the coefficients w_k we use the orthogonality condition

$$\sum_{m=0}^n {}'' \cos \frac{\pi i m}{n} \cos \frac{\pi j m}{n} = \begin{cases} 0 & \text{if } i \neq j, \\ n & \text{if } i = j = 0 \text{ or } n, \\ n/2 & \text{if } i = j \neq 0 \text{ or } n. \end{cases} \quad (3.3.3)$$

Let $t_m = \cos \frac{\pi m}{n}$. Then after multiplying both sides of (3.3.2) by $\cos \frac{\pi m k}{n}$, we get

$$\begin{aligned} \sum_{m=0}^n {}'' f(t_m) \cos \frac{\pi m k}{n} &= \sum_{m=0}^n {}'' \sum_{k=0}^n {}'' w_k T_k(t_m) \cos \frac{\pi m k}{n} \\ &= \sum_{m=0}^n {}'' \sum_{k=0}^n {}'' w_k \cos \frac{\pi k m}{n} \cos \frac{\pi k m}{n} = \frac{n}{2} w_k, \end{aligned}$$

which implies that w_k can be computed from the formula

$$w_k = \frac{2}{n} \sum_{m=0}^n {}'' f_m \cos \frac{\pi k m}{n}, \quad f_m = f\left(\cos \frac{\pi m}{n}\right). \quad (3.3.4)$$

Next, we use the result $\int_{-1}^1 T_k(x) dx = \begin{cases} 2/(1-k^2), & k \text{ even,} \\ 0, & k \text{ odd,} \end{cases}$ (see §1.3) to yield the *Clenshaw-Curtis rule*

$$\begin{aligned} I_{-1}^1(f) &= I_n(f) + E_n = \sum_{k=0}^n {}'' w_k f\left(\frac{k\pi}{n}\right) \\ &= \frac{4}{n} \sum_{m=0}^n {}'' f_m \sum_{k=0}^n {}'' \left\{ \begin{array}{ll} \frac{1}{1-k^2} \left(\cos \frac{\pi m k}{n}\right), & k \text{ even} \\ 0, & k \text{ odd} \end{array} \right. + E_n. \end{aligned} \quad (3.3.5)$$

This rule is exact if $f \in \mathcal{P}_{2n-1}$.

To generate this rule, Clenshaw and Curtis (1960) start with the expansion of $f(x)$ in terms of the Chebyshev polynomials of the first kind $T_n(x)$:

$$f(x) = \sum_{j=0}^{\infty} b_j T_j(x). \quad (3.3.6)$$

Then

$$\begin{aligned} \int_{-1}^1 f(x) dx &= \sum_{j=1}^{\infty} {}' b_j \int_{-1}^1 T_j(x) dx = \sum_{j=1}^{\infty} {}' b_j \int_0^{\pi} \cos j\theta \sin \theta d\theta \\ &= \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} {}' \frac{2b_n}{1-n^2}, \end{aligned} \quad (3.3.7)$$

where the coefficients b_j are given by

$$b_j = \frac{2}{\pi} \int_{-1}^1 \frac{f(x) T_j(x)}{\sqrt{1-x^2}} dx. \quad (3.3.8)$$

These coefficients can be computed by using the closed Gauss-Chebyshev rule; thus, from (3.3.8) we get

$$b_j \approx a_j(n) = \frac{2}{n} \sum_{k=0}^n {}'' f\left(\cos \frac{k\pi}{n}\right) \cos \frac{j\pi}{n}, \quad j = 0, 1, \dots, n, \quad (3.3.9)$$

Then the Clenshaw-Curtis rule is carried out in two steps:

(i) Compute $a_j^{(n)}$ for $j = 0, 1, \dots, n$ from (3.3.9). We need only the coefficients with even indices;

$$(ii) \text{ Compute } If = \sum_{\substack{j=0 \\ n \text{ even}}}^n {}'' \frac{2a_j^{(n)}}{1-j^2}. \quad (3.3.10)$$

Note that the last term in (3.3.10) is halved so as to obtain the result identical to the original derivation. The term $a_j^{(n)}$ is usually very small. By combining the above two steps, we obtain

$$\begin{aligned} If &= \sum_{\substack{j=0 \\ j \text{ even}}}^n {}'' \frac{4}{(1-j^2)n} \cos \frac{jk\pi}{n} f\left(\cos \frac{k\pi}{n}\right) \\ &= \sum_{k=0}^n {}'' w_k f\left(\cos \frac{k\pi}{n}\right), \end{aligned} \quad (3.3.11)$$

where

$$w_k = \frac{4}{\pi} \sum_{\substack{j=0 \\ j \text{ even}}}^n {}'' \frac{1}{1-j^2} \cos \frac{jk\pi}{n}. \quad (3.3.12)$$

If the rule (3.3.11) is applied directly, the cost of its implementation is very high. A direct computation of (3.3.12) to compute w_k , $k = 0, 1, \dots, n$, comes to $(n+1)^2$ multiplications and additions, as compared to only $(n+1)$ to compute (3.3.11) or (3.3.10). But since (3.3.9) has the form of a direct cosine transform, the coefficients w_k can be computed using FFT in $O(N \ln N)$ operations. The resulting rule is very stable and effective in cost. The above generation of the Clenshaw-Curtis rules, due to Imhof (1963), is based on the generalized Fourier expansion of the integrand $f(x)$ in terms of the Chebyshev polynomials $T_n(x)$.

O'Hara and Smith (1968) have studied the errors in the Clenshaw-Curtis rules. To obtain the error estimate, they integrate the generalized Fourier expansion of $f(x)$

$$f(x) = \sum_{k=0}^{\infty} {}' A_k T_k(x). \quad (3.3.13)$$

Let E_n denote the exact value of $I_{-1}^1(f)$ minus the value found by using the n -term approximation $I_n(f)$ in (3.3.11). Then comparing (3.3.13) and (3.3.4) we find that

$$\begin{aligned} w_k &= \frac{2}{n} \sum_{m=0}^n {}'' \cos \frac{\pi km}{n} \sum_{i=0}^{\infty} {}' A_i \cos \frac{\pi im}{n} \\ &= A_k + A_{2n-k} + A_{2n+k} + A_{4n-k} + A_{4n+k} + \dots \end{aligned} \quad (3.3.14)$$

Thus, from (3.3.5) we have two expressions, one for $I_n(f)$ and the other for $I_{-1}^1(f)$:

$$I_n(f) = w_0 - \frac{2w_2}{1 \cdot 3} - \frac{2w_4}{3 \cdot 5} - \cdots - \frac{2w_{n-2}}{(n-3)(n-1)} - \frac{w_n}{(n-1)(n+1)},$$

and

$$I_{-1}^1(f) = A_0 - \frac{2A_2}{1 \cdot 3} - \frac{2A_4}{3 \cdot 5} - \cdots,$$

which after subtraction give

$$\begin{aligned} E_n &= 2A_{2n} - \frac{2}{1 \cdot 3} (A_{2n-2} + A_{2n+2}) - \cdots \\ &\quad - \frac{2}{(n-3)(n-1)} (A_{n+2} + A_{3n-2}) \\ &\quad + \sum_{k=1}^{n-1} \frac{2A_{n+2k}}{(n+2k-1)(n+2k+1)}. \end{aligned} \quad (3.3.15)$$

Since $f(x)$ is assumed to be smooth, the coefficients A_k decrease more rapidly for large n , and therefore, we can ignore terms higher than A_{3n} . Also, we take n to be even. Then from (3.3.15) we find

$$\begin{aligned} E_n &= \sum_{k=0}^{n/2-1} \frac{2A_{2n-2k}}{4k^2-1} + \sum_{k=0}^{n/2-1} \frac{2A_{2n+2k}}{4k^2-1} \\ &\quad - \sum_{k=1}^{n-1} \frac{2A_{n+2k}}{(n+2k-1)(n+2k+1)}, \end{aligned}$$

which, after combining terms, where those in the first and third summations cancel, reduces to

$$\begin{aligned} E_n &= \frac{16 \cdot 1 \cdot n}{(n^2-1^2)(n^2-3^2)} A_{n+2} + \frac{16 \cdot 2 \cdot n}{(n^2-3^2)(n^2-5^2)} A_{n+4} \\ &\quad + \frac{16(n/2-1)n}{3(2n-1)(2n-3)} A_{2n-2} - \left(2 + \frac{2}{4n^2-1}\right) A_{2n} \\ &\quad + \left(\frac{2}{3} - \frac{2}{(2n+1)(2n+3)}\right) A_{2n+2} + \cdots. \end{aligned} \quad (3.3.16)$$

This expression clearly shows why the Clenshaw-Curtis rule is more accurate than its degree implies. The first two terms in (3.3.16) are dominant, but the factors multiplying A_{n+2} and A_{n+4} are of the order $1/n^2$, which make them very small, and therefore, provide better result with only a small sum. Thus, the Clenshaw-Curtis rule is very effective and numerically stable to high degree, like the other Gaussian rules. This rule is also self-contained since it does not require any tables for the weights

w_k , which makes it independent of the order of the formula to be used. This property enables the Clenshaw-Curtis rule to be operative on very small and portable computer systems. Gentleman (1972) uses fast cosine transform to implement this rule.

Another variation of the method for generating the Clenshaw-Curtis rule is due to Evans (1993b) and uses the trapezoidal rule in such a way that the error term in the Euler-Maclaurin summation formula (2.2.8) can be made zero. This method is realized by setting $x = \cos \theta$ in (3.3.8), which gives

$$b_j = \frac{2}{n} \int_0^\pi f(\cos \theta) \cos j\theta d\theta. \quad (3.3.17)$$

Then by applying the trapezoidal rule to (3.3.17) we obtain the approximation

$$b_j \approx \frac{2}{n} \left[\sum_{m=0}^n {}'' g\left(\cos \frac{\pi m}{n}\right) \cos \frac{\pi j m}{n} \right], \quad (3.3.18)$$

which is identical to (3.3.4). But the quadrature rules are not identical because in rule (3.3.5) the summation is \sum'' , whereas in rule (3.3.7) it is \sum' . However, for smooth integrands the rules will converge rapidly and the above difference in the last term will almost vanish in terms of computational accuracy.

A completely complementary set of quadrature rules of the Clenshaw-Curtis type is based on the use of an expansion of the integrand $f(x)$ as

$$f(x) = \sum_{k=0}^n c_k T'_k(x) + E_n, \quad (3.3.19)$$

where, after setting $x = \cos \theta$, we have $T'_k(x) = \frac{k \sin k\theta}{\sin \theta} = k U_k(x)$. We use the orthogonality relation

$$\sum_{m=0}^n {}'' \sin \frac{mi\pi}{n} \sin \frac{mj\pi}{n} = \begin{cases} 0 & \text{if } i \neq j, \\ n/2 & \text{if } i = j \neq 0 \text{ or } n, \\ n & \text{if } i = j = 0 \text{ or } n, \end{cases}$$

to determine the coefficients c_k in (3.3.19) in the same manner as in (3.3.4), and we find that

$$c_k = \frac{2}{jn} \sum_{m=0}^n {}'' f\left(\cos \frac{\pi m}{n}\right) \sin \frac{\pi m}{n} \sin \frac{\pi j m}{n}, \quad (3.3.20)$$

which yields

$$I_{-1}^1(f) \approx I_n(f) = \sum_{k=1}^n c_k \begin{cases} 2 & k \text{ even}, \\ 0 & k \text{ odd}. \end{cases} \quad (3.3.21)$$

Alternatively, for the approximation (3.3.19) we have

$$\begin{aligned} c_k &= \frac{2}{\pi k^2} \int_{-1}^1 f(x) T_k''(x) \sqrt{1-x^2} dx \\ &= \frac{2}{\pi k} \int_0^\pi f(\cos \theta) \sin \theta \sin k\theta d\theta. \end{aligned} \quad (3.3.22)$$

Another variation of (3.3.22) is obtained by applying the Gauss-Chebyshev quadrature rule to obtain the requisite weight $(1-x^2)^{-1/2}$. Then the formula

$$c_k = \frac{2}{\pi k^2} \int_{-1}^1 \frac{f(x) T_k'(x) (1-x^2)}{\sqrt{1-x^2}} dx$$

gives

$$c_k = \frac{2}{nk} \sum_{m=1}^n f(\cos \theta_m) \sin k\theta_m \sin \theta_m,$$

where $\theta_m = \frac{(2m-1)\pi}{2n}$. This yields

$$I_n(f) = \sum_{k=1}^n c_k \begin{cases} 2 & \text{if } k \text{ even,} \\ 0 & \text{if } k \text{ odd.} \end{cases}$$

which is the same as (3.3.21). Further, the relation (3.3.20) can be obtained by using (3.3.22) directly with the trapezoidal rule.

The Clenshaw-Curtis rules arise when we incorporate the endpoints -1 and 1 as nodes in the Fejér's $(2n-2)$ -point rule (see (3.2.15)). Thus, the nodes in the Clenshaw-Curtis rule are at $x_i = \cos\left(\frac{(i-1)\pi}{n-1}\right)$ for $i = 1, \dots, n$, and the weights at these nodes are given by

$$\begin{aligned} w_1 = w_n &= \begin{cases} \frac{1}{(n-1)^2} & \text{if } n \text{ is even,} \\ \frac{1}{n(n-2)} & \text{if } n \text{ is odd,} \end{cases} \\ w_i &= \left[1 - \sum_{j=1}^{[(n-1)/2]} \frac{2}{4j^2-1} \cos\left(\frac{2j(i-1)\pi}{n-1}\right) \right], \quad i = 1, \dots, n-1, \end{aligned}$$

where \sum^* means that the last term in the sum is halved if n is odd.

Piessens and Branders (1983) have applied a modified Clenshaw-Curtis rule to compute the integrals of the form $I_a^b(kf)$, where $k(x)$ is one of the singular functions $(x-a)^\alpha$, $(x-a)^\alpha \ln(x-a)$, $(b-x)^\alpha$, and $(b-x)^\alpha \ln(b-x)$, where $\alpha > -1$. They

do it by first approximating $f(x)$ by a Chebyshev series $f(x) \simeq \sum_{i=0}^n c_i T_i(x)$. Then $I_a^b(kf) \simeq \sum_{i=0}^n c_i M_i(x)$, where M_i are the modified moments of $k(x)$ with respect to the Chebyshev polynomials $T_i(x)$ and can be computed by recurrence formulas (see §4.4.10).

3.3.2. Gauss-Kronrod Rule. The Gauss formulas do not reuse the function values computed previously because these rules do not have any common nodes (quadrature points), except, possibly, the midpoint of the interval of integration, and thus, they do not allow the reuse of previous f -values. Kronrod (1965) devised a method by which an n -point Gaussian formula $K_n(f) = \sum_{k=1}^n w_k f(x_k)$ with n preassigned nodes is used to construct a $(2n+1)$ -point formula in such a way that the resulting formula possesses a high degree of accuracy, which is $3n+1$ for n even, and $3n+2$ for n odd. Since the n nodes are preassigned, the remaining $n+1$ nodes are located in the intervals $(a, x), (x_1, x_2), \dots, (x_n, b)$, where x_1, x_2, \dots, x_n denote the preassigned nodes of K_n .

The linear Gaussian rule

$$\int_a^b f(x) dx \approx G_n(f) = \sum_{i=1}^n w_i f(a + (b-a)x_i), \quad (3.3.23)$$

where $w_i, w_i \neq 0$, are the weights and x_i the nodes of the quadrature, is unique, and its accuracy is $2n-1$; i.e., this rule is accurate if $f \in \mathcal{P}_{2n-1}$. Note that the integral

$\int_a^b f(x) dx$ reduces to $\frac{b-a}{2} \int_{-1}^1 f(x(t)) dt$ by the substitution $t = 2\frac{x-a}{b-a} - 1$.

Kronrod uses the Legendre polynomials $L_n(x)$ of degree n which are orthogonal on $[-1, 1]$ (see §1.3). Then any polynomial of degree not higher than $2n-1$ is also integrable by formula (3.3.23), since any such polynomial can be represented in the form

$$P_{n-1}(x) + \sum_{k=0}^{n-1} C_k x^k L_n(x), \quad (3.3.24)$$

where $P_{n-1}(x)$ is a polynomial of degree not higher than $n-1$. Since each term in (3.3.24) is integrable accurately by the Gaussian rule $G_n(f)$, the sum is also so integrable, and therefore it has accuracy $2n-1$.

To construct another quadrature with maximum possible accuracy, Kronrod considers the k -th moment of the polynomial $L_n(x)$, which is defined by

$$K_{n,k} = \int_{-1}^1 L_n(x) x^k dx.$$

We set $P_{n+1}(x) = x^{n+1} + p_n x^n + p_{n-1} x^{n-1} + \dots + p_0$. Since $L_n(x)$ is orthogonal

on $[-1, 1]$ to all powers of x^k for $k < n$, we have

$$\begin{aligned} \int_{-1}^1 L_n(x) P_{n+1}(x) &= \int_{-1}^1 L_n(x) [x^{n+1} + p_n x^n + p_{n-1} x^{n-1} + \cdots + p_0] \, dx \\ &= M_{n,n+k+1} + p_n M_{n,n+k} + \cdots + p_{n-k} M_{n,n}, \quad k = 0, 1, \dots, n. \end{aligned}$$

This yields a recurrence formula for p_k :

$$\begin{aligned} p_{n+1} &= 1, \\ p_n &= -\frac{M_{n,n+1}}{M_{n,n}}, \\ p_{n-1} &= -\frac{M_{n,n+2} p_{n+1}}{M_{n,n} p_n}, \\ &\dots\dots\dots, \\ p_{n-k} &= -\frac{M_{n,n+1} p_{n+1} + \cdots + M_{n,n+1} p_{n-k+1}}{M_{n,n} p_n}, \\ &\dots\dots\dots \end{aligned}$$

Using this relation, we compute the moments $M_{n,k}$ by the formula

$$M_{n,n+2k} = M_{n,n+2k-2} \left(1 + \frac{\left\lfloor \frac{n}{2} \right\rfloor}{k} \right) \cdot \frac{2 \left\lfloor \frac{n+1}{2} \right\rfloor + 2k - 1}{2n + 2k + 1}.$$

Kronrod (1965) develops a modified Gaussian formula

$$K_n(f) \approx \sum_{i=1}^{2n+1} W_i f(x_i), \tag{3.3.25}$$

which has an accuracy of $3n+1$ for even n and of $3n+1$ for odd n . Table A.13 contains the nodes x_i and weights w_i or W_i for the formula $G_n(f)$ or $K_n(f)$, respectively, for $n = 1(1)5$; extensive tables are available in Kronrod (1965) for $n = 1, \dots, 40$ in decimal form (and $n = 1, \dots, 50$ in octal form) for the interval $[0, 1]$.

EXAMPLE 3.3.1. (Kronrod 1965) To compute $\int_{2.1}^{7.3} f(x) \, dx$, note that $a = 2.1$, $b = 7.3$, so $b - a = 5.2$, and we use $n = 5$. Then, using Table A.13, we get

$$\begin{aligned} G_5(f) &= 5.2 \left[0.1184634425280945 \times f(2.1 + (5.2)(0.0469100770306680)) \right. \\ &\quad + 0.2393143352496833 \times f(2.1 + (5.2)(0.2307653449471585)) \\ &\quad + 0.2844444444444444 \times f(2.1 + (5.2)(0.5)) \\ &\quad + 0.2393143352496833 \times f(2.1 + (5.2)(0.7692346550528415)) \\ &\quad \left. + 0.1184634425280945 \times f(2.1 + (5.2)(0.99920426800474212)) \right]; \end{aligned}$$

$$\begin{aligned}
K_5(f) = 5.2 & \left[0.0212910183755409 \times f(2.1 + (5.2)(0.079573199525788)) \right. \\
& + 0.0576166583112367 \times f(2.1 + (5.2)(0.0469100770306680)) \\
& + 0.0934008982782463 \times f(2.1 + (5.2)(0.1229166867145754)) \\
& + 0.1205201696143238 \times f(2.1 + (5.2)(0.2307653449471585)) \\
& + 0.1364249009562795 \times f(2.1 + (5.2)(0.601847934191084)) \\
& + 0.1414937089287456 \times f(2.1 + (5.2)(0.5)) \\
& + 0.1364249009562795 \times f(2.1 + (5.2)(0.6398152065808916)) \\
& + 0.1205201696143238 \times f(2.1 + (5.2)(0.7692346550528415)) \\
& + 0.0934008982782463 \times f(2.1 + (5.2)(0.8770833632854246)) \\
& + 0.0576166583112367 \times f(2.1 + (5.2)(0.9530899229693320)) \\
& \left. + 0.0212910183755409 \times f(2.1 + (5.2)(0.9920426800474212)) \right]. \blacksquare
\end{aligned}$$

A detailed discussion of Gauss-Kronrod rules is available in Piessens and Branders (1974).

3.3.3. Patterson's Rules. Unlike the Gauss-Kronrod rule, Patterson (1969) developed an alternative method of augmenting an n -point quadrature formula by p -points. The $n + p$ nodes of the new formula are zeros of the polynomial $G_{n+p}(x)$ yet to be determined. Then a general polynomial of degree $n + 2p - 1$ is written as

$$F_{n+2p-1}(x) = Q_{n+p-1}(x) + G_{n+p}(x) \sum_{k=0}^{p-1} c_k x^k, \quad (3.3.26)$$

where $Q_{n+p-1}(x) \in \mathcal{P}_{n+p-1}$ is a general polynomial. The polynomial $F_{n+2p-1}(x)$ defined in (3.3.26) is subjected to the constraint

$$\int_{-1}^1 G_{n+p}(x) x^k dx = 0, \quad k = 0, 1, \dots, p-1, \quad (3.3.27)$$

and it is then integrated exactly by an $(n + p)$ -point formula. This yields a rule with $(n + p)$ nodes. The constraint (3.3.27) can be generalized to

$$\int_{-1}^1 G_{n+p}(x) P_k(x) dx = 0, \quad k = 1, \dots, p-1, \quad (3.3.28)$$

where $P_k(x)$ are the Legendre polynomials. Then the polynomial $G_{n+p}(x)$ is expressed in terms of a series of Legendre polynomials

$$G_{n+p}(x) = \sum_{i=0}^{n+p} t_i P_i(x), \quad (3.3.29)$$

and substituting it into (3.3.28) yields

$$\sum_{i=0}^{n+p} t_i \int_{-1}^1 P_i(x) P_k(x) dx = 0, \quad k = 1, \dots, p-1. \quad (3.3.30)$$

In view of the orthogonality of the Legendre polynomials on $[-1, 1]$, Eq (3.3.30) implies that $t_i = 0$ for $i = 0, 1, \dots, p-1$. Hence, Eq (3.3.29) reduces to

$$G_{n+p}(x) = \sum_{i=p}^{n+p} t_i P_i(x),$$

which, in view of the symmetry of the nodes, is further simplified to

$$G_{n+p}(x) = \sum_{i=1}^{[n/2]+1} c_i P_{2i-2+p+q}(x), \quad q = n - 2[n/2]. \quad (3.3.31)$$

Without loss of generality, we choose $c_{[n/2]+1} = 1$. This leads to the following system of linear algebraic equations

$$\sum_{i=1}^{[n/2]} c_i P_{2i-2+p+q}(x_j) = -P_{n+p}(x_j), \quad j = 1, 2, \dots, [n/2], \quad (3.3.32)$$

which can be solved for the coefficients $c_1, c_2, \dots, c_{[n/2]}$. This determines the polynomials $G_{n+p}(x)$ completely as defined by (3.3.31), and thus the zeros of $G_{n+p}(x)$ make the set of extended nodes.

Morrow (1977) has noted that few such Patterson-type extensions of the Gaussian rule exist. The most commonly used rule is based on the 3-point Gauss-Legendre formulas, which has been extended to 7, 15, and 51 points. For practical purposes this rule is highly competitive with the Clenshaw-Curtis rule.

The nodes x_k and weights w_k for the Patterson quadrature rules 3, 7, 15, 31, 63 and 127 points, where the 3-point rule is the normal Gauss-Legendre rule, are presented in [Table A.14](#).

The NAG routine D01AHF provides an implementation of this rule, with the sequence of orders up to 255-point rule. If convergence is not attained at this limit, the subintervals are then halved, and the ϵ -algorithm (EPAL, see [Wynn 1956; algorithms.pdf](#) on the CD-R) is used to accelerate convergence.

Note that the Gauss-Kronrod Rule is a particular case of Patterson's quadrature rule with $p = 1$.

3.3.4. Basu Rule. This rule uses the relation $U_{n-1}(x) = \frac{1}{n} T'_n(x)$, where $T_n = \cos n\theta$, $x = \cos \theta$, is the Chebyshev polynomial of the first kind, and expands

a function $f(x)$ of bounded variation in $[-1, 1]$ in a series of $T'_n(x)$:

$$f(x) = \sum_{n=1}^{\infty} a_n T'_n(x), \quad (3.3.33)$$

where

$$a_n = \frac{2}{\pi n^2} \int_{-1}^1 (1-x^2)^{1/2} T'_n(x) f(x) dx. \quad (3.3.34)$$

In general, the weights in (3.3.34) cannot be evaluated, so the coefficients a_n are approximated by using the Filippi's quadrature scheme (Filippi 1964), which is as follows. Let $f(x)$ be approximated by a polynomial $p_{N-1}(x)$ over the zeros of $T'_{N+1}(x)$ so that

$$p_{N-1}(x) = \sum_{k=1}^N B_{k,N} T'_k(x), \quad (3.3.35)$$

where

$$B_{k,N} = \frac{2}{(N+1)k^2} \sum_{i=1}^N (1-x_i^2) T'_k(x_i) f(x_i), \quad x_i = \cos \frac{in}{N+1}, \quad i = 1(1)N. \quad (3.3.36)$$

Filippi's quadrature formula for (3.3.35) is

$$\int_{-1}^1 f(x) dx \approx \int_{-1}^1 p_{N-1}(x) dx = 2 \sum_{i=0}^M B_{2i+1,N} \quad (3.3.37)$$

where

$$M = \begin{cases} \frac{N-1}{2} & \text{if } N \text{ is odd,} \\ \frac{N-2}{2} & \text{if } N \text{ is even.} \end{cases}$$

Then substituting the values of $B_{2i+1,N}$ from (3.3.36) into (3.3.37) we obtain

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^N \lambda_i f(x_i), \quad (3.3.38)$$

where

$$\lambda_i = \frac{4}{N+1} \sum_{j=0}^M \frac{(1-x_i^2)}{(2j+1)^2} T'_{2j+1}(x_i).$$

The error in formula (3.3.38) for large N is

$$|E_{N-1}| \leq \frac{\sigma_{N,N+3}}{\rho^2 - 1} \frac{(\rho + \rho^{-1})^2}{\rho^{N+1} - \rho^{-(N+1)}} M(\rho),$$

where

$$\sigma_{N,N+3} = 2 \sum_{m=1}^{N+1} \frac{1}{2m+1},$$

$M(\rho)$ is a constant depending on ρ which is the radius of the circle where $f(z)$ is analytic. Thus, in this rule the nodes are at $x_1 = 1$, $x_n = -1$, and $x_i = \cos\left(\frac{(2i-3)\pi}{2n-2}\right)$ for $i = 2, \dots, n-1$. The weights in this rule are not all positive, but the sequence of sums of $|w_i|$ is uniformly bounded, and thus the Basu rule converges for all $f \in C[-1, 1]$.

EXAMPLE 3.3.2. (Basu 1970) Consider $\int_{-1}^1 dx/(x+4) = \ln(5/3) \approx 0.510825$. For $\rho = 7$ and $M(\rho) = 2.33333347$, the results for the error are as follows: For $N = 3$: $E = 1.66(-03)$; for $N = 5$: $E = 4.02(-05)$; for $N = 7$: $E = 9.3(-07)$; and for $N = 9$: $E = 2.0(-08)$. ■

3.4. Analytic Functions

Let $w \geq 0$ be the weight function on the interval $[-1, 1]$. To approximate $I_{-1}^1(wf)$, we use interpolatory quadrature formulas of the form

$$Q_n(f) = \sum_{k=1}^n w_{k,n} f(x_{k,n}), \quad (3.4.1)$$

where $-1 \leq x_{1,n} < x_{2,n} < \dots < x_{n,n} \leq 1$. If the integrand f is analytic in a simply connected and bounded region D of the complex plane containing $[-1, 1]$ in its interior, the remainder term $R_n(f) = I(wf) - Q_n(f)$ is given by

$$R_n(f) = \frac{1}{2i\pi} \int_{\Gamma=\partial D} K_n(z, w) f(z) dz,$$

where $K_n(z, w)$ is the kernel of the functional $R_n(f)$ (or of the quadrature rule $Q_n(f)$), and is given by

$$\begin{aligned} K_n(z, w) &= \frac{q_n(z)}{p_n(z)}, \\ p_n(z) &= c(z - x_{1,n}) \cdots (z - x_{n,n}), \\ q_n(z) &= \int_{-1}^1 w(x) \frac{p_n(z)}{z - x} dx \quad \text{for } z \in \mathbb{C} \setminus [-1, 1]. \end{aligned}$$

Alternatively,

$$K_n(z, w) = \int_{-1}^1 \frac{w(x)}{z - x} dx - \sum_{k=1}^n \frac{w_{k,n}}{z - x_{k,n}}.$$

The quadrature formula (3.4.1) has the error estimate

$$|R_n(f)| \leq \frac{l(\Gamma)}{2\pi} \max_{z \in \Gamma} |K_n(z, w)| \max_{z \in \Gamma} |f(z)|,$$

where $l(\Gamma)$ denotes the length of Γ . The contours Γ are generally taken as concentric circles centered at the origin or confocal ellipses \mathcal{E} with foci at ± 1 and defined by $\mathcal{E}_\rho = \frac{1}{2} [\rho e^{i\theta} + \rho^{-1} e^{-i\theta}]$, $0 \leq \theta < 2\pi$, $\rho \geq 1$. A good estimate of the bound for the error $R_n(f)$ is possible only if one can estimate $\max_{z \in \Gamma} |K_n(z, w)|$. For this purpose the location of the extremum of $|K_n|$ must be determined. It becomes easier to calculate $|K_n(z, w)|$ in the case when $Q_n(f)$ is a Gaussian rule. Gautschi and Varga (1983) have provided effective algorithms to calculate $|K_n(z, w)|$ at any point z outside $[-1, 1]$. The evaluation of the maximum point for $|K_n(z, w)|$ in the cases of circular or elliptic contours has been investigated by Gautschi and Li (1990), Gautschi (1991) and Peherstorfer (1993), where the results obtained in these studies deal with Chebyshev weights or for cases where $w(x)/w(-x)$ is monotone.

3.4.1. Symmetric Weight Functions. Let w be a symmetric weight on $[-1, 1]$, i.e., $w(-x) = w(x)$ for every $x \in [-1, 1]$. A generalized Gauss-Lobatto quadrature formula is (Hunter and Nikolov 1999)

$$Q_n^{(N)}(f) = \sum_{j=0}^{N-1} A_{j,n} \left[f^{(j)}(-1) + (-1)^j f^{(j)}(1) \right] + \sum_{k=1}^n w_{k,n}^{(N)} f(x_{k,n}^{(N)}), \quad (3.4.2)$$

where the remainder term $R_n^{(N)} = I(wf) - Q_n^{(N)}(f)$ is identically zero if $f \in \mathcal{P}_{2(n+N)-1}$. In particular, $Q_n^{(0)}(f)$ is the n -point Gaussian quadrature formula

$$Q_n^{(0)}(f) \equiv Q_n^G(f) = \sum_{k=1}^n w_{k,n}^G f(x_{k,n}^G); \quad (3.4.3)$$

$Q_n^{(1)}(f)$ is the $(n+2)$ -point Gauss-Lobatto quadrature formula

$$Q_n^{(1)}(f) \equiv Q_n^L(f) = A_n^L [f(-1) + f(1)] + \sum_{k=1}^n w_{k,n}^L f(x_{k,n}^L); \quad (3.4.4)$$

and $Q_n^{(2)}(f)$ is the $(n+2)$ -point Gauss-Lobatto quadrature formula with double end nodes, i.e., $Q_n^{(2)}(f) \equiv Q_n^{L,d}(f)$. The kernel $K_n^G(z, w)$ of formula (3.4.3) is evaluated on elliptic contours \mathcal{E}_ρ by Schira (1997). The intersection point of the ellipse \mathcal{E}_ρ with the positive branches of the real and imaginary axis is given by $z_r = \frac{\rho + \rho^{-1}}{2}$ and $z_i = \frac{i(\rho - \rho^{-1})}{2}$, respectively. It is found that for the weight function $w(x)$, symmetric on $[-1, 1]$, such that (i) $w(x)\sqrt{1-x^2} \uparrow$ on $[-1, 1]$, or (ii) $w(x)/\sqrt{1-x^2} \downarrow$ on

$[-1, 1]$ (i.e., $w(x)$ is the Gegenbauer weight function $w_\alpha(x) = (1 - x^2)^\alpha$, $\alpha > -1$, $\alpha \notin (-1/2, 1/2)$), the extremum of K_n^G coincides with z_r in the case (i) and with z_i in the case (ii), provided ρ is not less than some prescribed value which is given explicitly in the following cases.

If $w(x)\sqrt{1-x^2} \uparrow$ on $(0, 1)$, then

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^L(z, w)| = |K_{n+2}^L(z_r, w)| \quad \text{for all } \rho \geq \frac{1 + \sqrt{3}}{\sqrt{2}}. \quad (3.4.5)$$

For $n = 0$ this result is true for all $\rho > 1$.

The kernel $K_n^{(N)}(z, w)$ of formula (3.4.2) for a symmetric weight function $w(x)$ on $(-1, 1)$ is represented by

$$K_N^{(N)}(z, w) = (-1)^N \sum_{k=0}^{\infty} \frac{c_{n+2k+2}^{(N)}}{c_{n+2k}^{(N)}} \frac{z}{(z^2 - 1)^N \pi_{n+2k}^{(N)}(z) \pi_{2+2k+2}^{(N)}(z)}, \quad (3.4.6)$$

for $z \in \mathcal{C} \setminus [-1, 1]$, where $\pi_j^{(N)}$ is the j -th orthonormal polynomial with respect to the weight function $w^{(N)}(x) = (1 - x^2)^N w(x)$ and $c_j^{(N)}$ is its leading coefficient. For $N = 0$ and 1, the representation (3.4.6) is given in Schira (1997). Other useful results are:

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^L(z, w)| = |K_{n+2}^L(z_i, w)| \quad \text{for all } \rho \geq \begin{cases} 3.88 & \text{if } n \text{ is odd,} \\ 3.72 & \text{if } n \text{ is even;} \end{cases};$$

and

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^{L,d}(z, w)| = |K_{n+2}^{L,d}(z_r, w)| \quad \text{for all } \rho \geq \frac{1 + \sqrt{3}}{\sqrt{2}};$$

For the Gegenbauer weight function $w_\alpha(x) = (1 - x^2)^\alpha$, $\alpha > -1$, $\alpha \notin (-1/2, 1/2)$, we have

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^L(z, w_\alpha)| = \begin{cases} |K_{n+2}^L(z_r, w_\alpha)| & \text{if } -1 < \alpha \leq -1/2, \ n \geq 1, \\ |K_{n+2}^L(z_i, w_\alpha)| & \text{if } \alpha \geq 1/2, \ n \geq 3; \end{cases}$$

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^{L,d}(z, w_\alpha)| = |K_{n+2}^{L,d}(z_r, w_\alpha)| \quad \text{for all } \rho \geq \frac{1 + \sqrt{3}}{\sqrt{2}};$$

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^L(z, w_{-1/2})| = |K_{n+2}^L(z_r, w_{-1/2})| \quad \text{for all } \rho \geq 1;$$

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^L(z, w_{1/2})| = |K_{n+2}^L(z_i, w_{1/2})| \quad \text{for all } \rho \geq \rho(n);$$

$$\max_{z \in \mathcal{E}_\rho} |K_{n+2}^{L,d}(z, w_{-1/2})| = |K_{n+2}^{L,d}(z_r, w_{-1/2})| \quad \text{for all } \rho > 1,$$

where $\lim_{n \rightarrow \infty} \rho(n) = 1$. Some values of $\rho(n)$ are: $\rho(3) = 3.8318$, $\rho(4) = 3.2308$, $\rho(5) = 3.0022$, $\rho(6) = 2.8791$, $\rho(7) = 2.8000$, $\rho(8) = 2.7447$, $\rho(9) = 2.7036$,

$\rho(10) = 2.6718$, $\rho(11) = 2.6464$, $\rho(12) = 2.6256$, $\rho(13) = 2.6083$, $\rho(14) = 2.5937$, $\rho(15) = 2.5811$, $\rho(16) = 2.5702$, $\rho(17) = 2.5607$, $\rho(18) = 2.5522$, $\rho(19) = 2.5447$, $\rho(20) = 2.5380$, $\rho(21) = 2.5319$, $\rho(22) = 2.5264$, $\rho(23) = 2.5214$, $\rho(24) = 2.5168$, $\rho(25) = 2.5126$, $\rho(26) = 2.5087$, $\rho(27) = 2.5052$, $\rho(28) = 2.5019$, $\rho(29) = 2.4988$, $\rho(30) = 2.4959$, $\rho(60) = 2.4548$, $\rho(100) = 2.4385$.

3.4.2. Optimal Quadrature Rules. To generate quadrature rules of the highest degree of precision with arbitrarily preassigned nodes for general constant weight functions, Patterson (1989) considers the quadrature rule

$$I_a^b(wf) \approx \mathcal{R}(n, m) = \sum_{k=1}^n A_k f(x_k) + \sum_{k=1}^m A_{k+n} f(x_{k+n}), \quad (3.4.7)$$

where the n nodes x_1, \dots, x_n are preassigned, and the m nodes x_{n+1}, \dots, x_{n+m} , which are called the *optimally* added nodes, are free and are to be computed so as to achieve the highest degree of precision. As mentioned above, Kronrod (1965) computed tables of such rules; in fact, he took the n preassigned nodes as the zeros of $P_n(x)$ and used the Gauss-Legendre rule; he also computed additional $(n+1)$ additional nodes to provide all $2n+1$ nodes. These additional nodes are the zeros of a polynomial $\psi_{n+1}(x)$ such that $\int_{-1}^1 x^n P_n(x) \psi_{n+1}(x) dx = 0$ for $k = 0, \dots, n$. Let $\phi_i(x)$, $i = 1, 2, \dots$, denote a set of polynomials orthogonal on the interval $[a, b]$ with respect to a constant weight function $w(x)$, where $\int_a^b w(x) \phi_i(x) \phi_j(x) dx = h_j \delta_{ij}$ defines the j -th moment integral, where δ_{ij} is the Kronecker delta, such that

$$\phi_{n+1} = (c_k x + d_k) \phi + e_k \phi_{k-1}, \quad (3.4.8)$$

with $\phi_{-1} = 0$, $\phi_0 = 1$, where $e_k c_{k-1} h_{k-1} = -c_k h_k$. This yields

$$\frac{h_k}{h_0} = (-1)^k \frac{c_0}{c_k} \prod_{i=1}^k e_i.$$

To construct an $(n+m)$ mode quadrature rule which has n preassigned nodes, let these preassigned nodes be the zeros of a polynomial $q_n(x)$, where

$$q_n(x) = \sum_{i=m_0}^n \frac{\tau_i}{h_i} \phi_i(x),$$

and let $p_m(x) = \sum_{i=0}^m \varepsilon_m \phi_i(x)$ be the polynomial to be determined with the m additional nodes. Patterson (1989) proves that $\mathcal{R}(n, m)$, defined by (3.4.7), has the integrating degree $n + 2m + \mu - 1$, where $\mu > 0$, and that the quadrature weights associated with the s optimal nodes of the rule $\mathcal{R}(n+m, s)$ corresponding to the

extension of $\mathcal{R}(n, m)$ is zero unless $s > m + \mu$, $\mu > 0$. If $\mu = 0$, the orthogonality is nondegenerate.

The polynomials $p_m(x)$ are computed as follows. If

$$q_{n+m}(x) = q_n(x) p_m(x) = \sum_{j=0}^m \varepsilon_j \sum_{i=m_0}^n \frac{\tau_i}{h_i} \phi_i \phi_j = \sum_{j=0}^{n+m} \frac{\rho_j}{h_j} \phi_j, \quad (3.4.9)$$

then $\rho_j = 0$, $j = 0, \dots, m-1$, implies that $q_n(x) p_m(x) = \sum_{j=m}^{n+m} \frac{\rho_j}{h_j} \phi_j$. The coefficients ε_i of $p_m(x)$ are computed from (3.4.9).

Since it is computationally expensive to generate new Gaussian formulas, there are only a few commonly used combinations of intervals and weight functions available for well-known Gaussian rules. These combinations are available in Table 1.3.1. However, the above Patterson's method and the related algorithm can be used to produce specific individual quadrature rules or sequences of rules by iterative application of this method with all its details and algorithm presented in Patterson (1989). A method to reduce the number of coefficients necessary to represent Patterson's quadrature formulas, to reduce the amount of storage of computed function values, and to produce slightly smaller errors is presented by Krough and Van Snyder (1991).

3.5. Bessel's Rule

To compute $I(f) = \int_a^b f(x) dx$ numerically, we have *Bessel's rule* (see [Stummel and Hainer 1982](#), p. 75):

$$B(f) = \frac{b-a}{24} [-f(a-h) + 13f(a) + 13f(b) - f(b+h)]. \quad (3.5.1)$$

This integration uses nodes outside the integration interval. Garloff et al. (1986) derive three new rules. Let $[a, b]$ be a finite interval, and $f \in C^3[c, d]$, $c < a < b < d$. To compute $I(f)$ choose the nodes $x_i = a + ih$, $i = 0, 1, \dots, n$, and $h = (b-a)/n$. Assume that $c < a - h/6$ and $b + h/6 < d$, and let $f_0 = f(x_0)$, $f'_0 = f'(x_0), \dots$. Then let

$$I_1 = \int_{x_0}^{x_1} f(x) dx = hf_0 + \frac{h^2}{2!} f'_0 + \frac{h^3}{3!} f''_0 + \frac{h^4}{4!} f'''(\xi), \quad x_0 < \xi < x_1. \quad (3.5.2)$$

Replace $f(x)$ by a linear function $\phi(x) = f_0 + \alpha(x - x_0)$. Then

$$\tilde{I}_1 = \int_{x_0}^{x_1} \phi(x) dx = hf_0 + \frac{h^2}{2} \alpha.$$

We set $\alpha = \frac{1}{h} [f(x_0 + p_1 h) - f(x_0 + p_2 h)]$, where we determine p_1, p_2 so that (3.5.2) and the Taylor's expansion of \tilde{I}_1 coincide in the highest possible degree. Expanding α , we have

$$\alpha = f'_0(p_1 - p_2) + \frac{h}{2}(p_1^2 - p_2^2) + \frac{h^2}{6}[f'''(\xi_1)p_1^3 - f'''(\xi_2)p_2^3],$$

where $x_0 < \xi_j < x_0 + p_j h$, $j = 1, 2$, then, substituting this into \tilde{I}_1 , we get

$$\tilde{I}_1 = hf_0 + \frac{h^2}{2}f'_0(p_1 - p_2) + \frac{h^3}{4}f''_0(p_1^2 - p_2^2) + \frac{h^4}{12}[f'''(\xi_1)p_1^3 - f'''(\xi_2)p_2^3],$$

which yields $I_1 - \tilde{I}_1 = O(h^4)$ if $p_1 - p_2 = 1$ and $p_1^2 - p_2^2 = 2/3$, i.e., if $p_1 = 5/6$ and $p_2 = -1/6$. Then

$$\tilde{I}_1 = h \left[f(x_0) + \frac{1}{2} \left\{ f(x_0 + 5h/6) - f(x_0 - h/6) \right\} \right].$$

Similarly, for other subintervals $[x_i, x_{i+1}]$, $i = 1, 2, \dots, n-1$, we have

$$\tilde{I}_{i+1} = h \left[f(x_i) + \frac{1}{2} \left\{ f(x_i + 5h/6) - f(x_i - h/6) \right\} \right].$$

Using the relation $f(x_i + 5h/6) = f(x_{i+1} - h/6)$, we obtain the quadrature formula

$$\begin{aligned} \tilde{I}(f) &= \sum_{i=1}^n \tilde{I}_i \\ &= h \left[\sum_{i=0}^{n-1} f(x_i) + \frac{1}{2} \left\{ f(x_n - h/6) - f(x_0 - h/6) \right\} \right]. \end{aligned} \quad (3.5.3)$$

A related quadrature formula is

$$\tilde{J}(f) = h \left[\sum_{i=0}^n f(x_i) + \frac{1}{2} \left\{ f(x_0 + h/6) - f(x_n + h/6) \right\} \right]. \quad (3.5.4)$$

Finally, set

$$\begin{aligned} Q(f) &= \frac{1}{2} [\tilde{I}(f) + \tilde{J}(f)] = h \left[\sum_{i=0}^{n-1} f(x_i) + \frac{1}{2} \{ f(x_0) + f(x_n) \} \right. \\ &\quad \left. + \frac{1}{4} \{ f(x_0 + h/6) - f(x_0 - h/6) + f(x_n - h/6) - f(x_n + h/6) \} \right]. \end{aligned} \quad (3.5.5)$$

Thus, $Q(f)$ is equal to a *compound trapezoidal rule*

$$T_n(f) = h \left[\sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} \{f(x_0) + f(x_n)\} \right],$$

with the “end correction.” Since $T_n(f)$ is a Riemann sum, we get $Q(f) \rightarrow I(f)$ as $n \rightarrow \infty$ for all functions $f \in R[a, b]$ provided that the end correction tends to zero as $n \rightarrow \infty$. Now, we compare the formulas (3.5.3)–(3.5.5) to some other quadrature formulas. Thus,

(i) If $Z(f)$ denotes a quadrature formula, define $R_m^Z(f) = I(f) - Z(f)$, where m represents the number of function evaluations needed to compute $Z(f)$. The following error estimates hold:

$$\begin{aligned} |R_{n+2}^{\tilde{I}}(f)| &\leq (0.01105583 - 0.0017039/n) h^3(b-a) \sup_{x \in [a-h/6, b]} |f'''(x)|, \\ |R_{n+2}^{\tilde{J}}(f)| &\leq (0.01105583 - 0.0017039/n) h^3(b-a) \sup_{x \in [a, b+h/6]} |f'''(x)|, \\ |R_{n+5}^Q| &\leq c_k h^k(b-a) \sup_{x \in [a-h/6, b+h/6]} |f^{(k)}(x)|, \end{aligned}$$

for $f \in C^k[a-h/6, b+h/6]$, $k = 1, 2, 3, 4$, where $c_1 = \frac{1}{4}$, $c_2 = \frac{\sqrt{3}}{54}$, $c_3 = \frac{1}{192} + \frac{1}{1296n}$, and $c_4 = \frac{23}{12960}$.

(ii) For the compound Simpson's rule (n even):

$$\begin{aligned} S(f) &= \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots \\ &\quad + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)], \end{aligned}$$

the error estimates are

$$|R_{n+1}^S(f)| \leq d_k h^k(b-a) \sup_{x \in [a, b]} |f^{(k)}(x)|,$$

for $f \in C^k[a, b]$, $k = 1, 2, 3, 4$, and $d_1 = 5/18$, $d_2 = 4/81$, $d_3 = 1/72$, and $d_4 = 1/180$. If we compare (i) and (ii), we find that $c_k < d_k$ for $k = 1, 2, 3, 4$.

(iii) For the compound two-point and three-point Gaussian rules (n even):

$$\begin{aligned} G_2(f) &= h \sum_{i=1}^{n/2} [f(x_{2i-1} - h_2) + f(x_{2i-1} + h_2)], \\ G_3(f) &= \frac{h}{9} \sum_{i=1}^{n/2} [5f(x_{2i-1} - h_3) + 8f(x_{2i-1}) + 5f(x_{2i-1} + h_3)], \end{aligned}$$

with $h_2 = h/\sqrt{3} \approx 0.5773503 h$ and $h_3 = h/\sqrt{5} \approx 0.7745967 h$, the error estimates are

$$\begin{aligned} |R_n^{G_2}| &\leq \frac{1}{270} h^4(b-a) \sup_{x \in [a,b]} |f^{(4)}(x)|, \quad \text{for } f \in C^4[a, b], \\ |R_{3n/2}^{G_3}| &\leq \frac{1}{31500} h^6(b-a) \sup_{x \in [a,b]} |f^{(6)}(x)|, \quad \text{for } f \in C^6[a, b]. \end{aligned}$$

(iv) For the compound Bessel's rule

$$\begin{aligned} B(f) = h \left[\frac{1}{2} f(x_0) + f(x_1) + \dots + f(x_{n-1}) + \frac{1}{2} f(x_n) \right. \\ \left. + \frac{1}{24} \{ -f(x_0 - h) + f(x_1) + f(x_{n-1}) - f(x_n + h) \} \right], \end{aligned}$$

the error estimate is

$$|R_{n+3}^B(f)| \leq \frac{11}{720} h^4(b-a) \sup_{x \in [a-h, b+h]} |f^{(4)}(x)| \quad \text{for } f \in C^4[a-h, b+h].$$

3.5.1. Extrapolation. The Euler-Maclaurin formula (2.2.8) gives an expansion of the error of the compound trapezoidal rule T in terms of the step size h as follows: for $f \in C^{2n}[a, b]$,

$$\begin{aligned} I(f) = T(f) + r_1 h^2 + r_2 h^4 + \dots + r_{n-1} h^{2n-2} + E_1(f), \\ r_j = \frac{B_{2j}}{(2j)!} \left[f^{(2j-1)}(a) - f^{(2j-1)}(b) \right], \quad j = 1, 2, \dots, n-1, \end{aligned} \quad (3.5.6)$$

where B_j are the Bernoulli numbers, and $E_1(f) = O(h^{2n})$. Using Taylor's expansion, we have

$$\begin{aligned} T(f) - \tilde{I}(f) = -\frac{h^2}{2 \cdot 6} [f'(a) - f'(b)] + \frac{h^3}{2 \cdot 2! 6^2} [f''(a) - f''(b)] \\ - \dots + \frac{h^{2n}}{2(2n-1)! 6^{2n-1}} \left[f^{(2n-1)}(\eta_1) - f^{(2n-1)}(\eta_2) \right], \end{aligned}$$

where $\eta_1 \in (a - h/6, a)$ and $\eta_2 \in (b - h/6, b)$. Substituting this in (3.5.6), we get

$$\begin{aligned} I(f) = \tilde{I}(f) + s_2 h^2 + s_3 h^3 + \dots + s_{2n-1} h^{2n-1} + E_2(f), \\ s_{2k} = \left[\frac{B_k}{(2k)!} + \frac{1}{2(2k-1)! 6^{2k-1}} \right] \left[f^{(2k-1)}(a) - f^{(2k-1)}(b) \right], \\ s_{2k+1} = \frac{f^{(2k)}(a) - f^{(2k)}(b)}{2(2k)! 6^{2k}}, \quad k = 1, 2, \dots, n-1, \end{aligned}$$

where $E_2(f) = O(h^{2n})$. Similarly, for $\tilde{J}(f)$ we have

$$\begin{aligned} I(f) = \tilde{J}(f) + t_2 h^2 + t_3 h^3 + \dots + t_{2n-1} h^{2n-1} + E_3(f), \\ t_{2k} = s_{2k}, \quad t_{2k+1} = -s_{2k+1}, \quad k = 1, 2, \dots, n-1, \end{aligned}$$

where $E_3(f) = O(h^{2n})$. Combining these two, we find that

$$I(f) = Q(f) + s_4 h^4 + s_6 h^6 + \cdots + s_{2n-2} h^{2n-2} + E_4(f),$$

where $E_4(f) = O(h^{2n})$. Now, we consider quadrature rules for \tilde{I} , \tilde{J} , and Q for successively halving the step size h with $h_j = 2^{-j}h$, $n_j = 2^j n$, and applying extrapolation, we get

$$\begin{aligned}\tilde{I}(f) &= h_j \left[\sum_{i=0}^{n_j-1} f(x_0) + \frac{1}{2} \{f(b - h_j/6) - f(a - h_j/6)\} \right], \\ \tilde{J}(f) &= h_j \left[\sum_{i=0}^{n_j} f(x_0) + \frac{1}{2} \{f(a + h_j/6) - f(b + h_j/6)\} \right], \\ Q_j(f) &= \frac{1}{2} [\tilde{I}_j(f) + \tilde{J}_j(f)],\end{aligned}$$

Define for $k = 0, 1, \dots, j-1$,

$$\begin{aligned}\tilde{I}_j^0 &= \tilde{I}_j(f), & \tilde{I}_j^{k+1}(f) &= (2^{k+3} - 1)^{-1} [2^{k+3} \tilde{I}_{j+1}^k(f) - \tilde{I}_j^k(f)], \\ \tilde{J}_j^0 &= \tilde{J}_j(f), & \tilde{J}_j^{k+1}(f) &= (2^{k+3} - 1)^{-1} [2^{k+3} \tilde{J}_{j+1}^k(f) - \tilde{J}_j^k(f)], \\ Q_j^0 &= Q_j(f), & Q_j^{k+1}(f) &= (2^{k+3} - 1)^{-1} [(2^{2k+4} Q_{j+1}^k(f) - Q_j^k(f))].\end{aligned}$$

Then for each $f \in C^{2n}[c, d]$, we have

$$\begin{aligned}I(f) &= \tilde{I}_j^k(f) + \sum_{m=k}^{2n-4} s_{m+3}^k h_j^{m+3} + O(h_j^{2n}), \quad k \leq 2n-4, \\ I(f) &= Q_j^k(f) + \sum_{m=k}^{n-3} u_{2m+4}^k h_j^{2m+4} + O(h_j^{2n}), \quad k \leq n-3,\end{aligned}$$

with suitably chosen constants s_{m+3}^k and u_{2m+4}^k . Similar expression are obtained for $\tilde{J}^k(f)$.

Garloff et al. (1986) have considered the following examples numerically.

1. $\int_0^\pi \cos(\sin x - x) dx \approx 1.38246,$
2. $\int_0^1 4(x^2 + 1)^{-1} dx = \pi,$
3. $\int_0^{\pi/2} (1 - 0.81 \sin^2 \phi)^{-1/2} d\phi \approx 2.28055,$

$$\begin{aligned}
4. \quad & \int_0^2 e^{-x^2} dx \approx 0.88208, \\
5. \quad & \int_0^{\pi/2} \sqrt{\cos x} dx \approx 1.19814.
\end{aligned}$$

The Bessel's rule \tilde{I} and Q will not be applicable in 5 if the integration limits contain the interval $(\pi/2, 3\pi/2)$, because the factor $\sqrt{\cos x}$ is not real in this interval.

3.5.2. Nodes inside the Integration Interval. The formulas \tilde{I} , \tilde{J} and Q use nodes outside the integration interval. Now, we derive fourth-order formulas (see [Ralston 1959](#)) which use nodes inside the integration interval.

If we replace the integrand $f(x)$ by a linear function $\phi(x) = f(qh) + \alpha(x - qh)$, $0 \leq q \leq 1$, and use Taylor's expansion about qh , we get

$$I(f) \approx h \left[f(qh) + \left(\frac{1}{2} - q\right) \{f((q + p_1)h) - f((q + p_2)h)\} \right], \quad (3.5.7)$$

where p_1, p_2 depend on q . As in the previous section, the only choice of p_1 and p_2 such that $0 \leq p_k + q \leq 1$, $k = 1, 2$, and (3.5.7) to be of order 4 is $p_k = \frac{1}{2} [1 + (-1)^k 3^{-1/2}]$ for $k = 1, 2$. For these values of p_1 and p_2 we have

$$I(f) \approx V_k(f) = h \left[f\left(\frac{h}{2} \left(1 + (-1)^k 3^{-1/2}\right)\right) - \frac{(-1)^k 3^{-1/2}}{2} \{f(h) - f(0)\} \right].$$

If we take the arithmetic mean of both of these approximations, we obtain the two-point Gaussian rule. The above basic rule $V_k(f)$ leads to the following compound rule for $k = 1, 2$:

$$V_{k,n+2}(f) = h \left[\sum_{i=0}^{n-1} f\left(ih + \frac{h}{2} (1 + (-1)^k 3^{-1/2})\right) - \frac{1}{2} (-1)^k 3^{-1/2} \{f(nh) - f(0)\} \right]. \quad (3.5.8)$$

The third Peano kernel of V_k is given by

$$K_3^k(x) = \begin{cases} \frac{x^2}{6} [(-1)^k 3^{-1/2} \frac{h}{2} - x] & \text{if } 0 \leq x \leq \frac{h}{2} (1 + (-1)^k 3^{-1/2}), \\ \frac{(x-h)^2}{12} [(2 + (-1)^k 3^{-1/2})h - 2x] & \text{if } \frac{h}{2} (1 + (-1)^k 3^{-1/2}) \leq x \leq h, \end{cases}$$

and for $k = 1, 2$ we have

$$\int_0^h K_3^k(x) dx = (-1)^k \frac{h^4 \sqrt{3}}{216}. \quad (3.5.9)$$

Since $(-1)^k K_3^k(x) > 0$ for $x \in (0, h)$, we find from (3.5.9) that the error in the compound rule (3.5.8) is

$$I(f) - V_{k,n+2}(f) = (-1)^k 3^{-1/2} \frac{h^3 b}{216} f'''(\theta_k), \quad \theta_k \in [0, h], \quad k = 1, 2. \quad (3.5.10)$$

If $(-1)^k f'''(x) \geq 0$ for all $x \in [0, h]$, then (3.5.10) yield

$$(-1)^k V_{2,n+2}(f) \leq (-1)^k I(f) \leq (-1)^k V_{1,n+2}(f) \quad \text{for } k = 1, 2. \tag{3.5.11}$$

When successively halving the step size, the left and right side of the inequality (3.5.11) increase and decrease. Since this monotone behavior holds for a wide class of quadrature rules, we define it for an arbitrary basic quadrature rule $Z(f)$:

$$Z(f) = \sum_{i=0}^n \alpha_i f(\beta_i), \quad \beta_i \in [a, b], \tag{3.5.12}$$

which is exact for $f \in \mathcal{P}_{s-1}$. Denote the associated compound rule with respect to the step size h by $Z_h(f)$ and define

$$Z_{h/2,h}^{(s)}(x) = Z_{h/2} \left[\frac{(t-x)_+^{s-1}}{(s-1)!} \right] - Z_h \left[\frac{(t-x)_+^{s-1}}{(s-1)!} \right], \tag{3.5.13}$$

where $(t-x)_+^{s-1} = \begin{cases} (t-x)^{s-1} & \text{if } t \geq x, \\ 0 & \text{if } t < x \end{cases}$. Then, if $f \in C^s[a, b]$, we have

$$Z_{h/2}(f) - Z_h(f) = \int_a^b f^{(s)}(x) Z_{h/2,h}(x) dx. \tag{3.5.14}$$

Hence, we conclude that if $f'''(x) \leq 0$ for all $x \in [a, b]$, then

$$V_{1,3}(f) \leq V_{1,4}(f) \leq V_{1,6}(f) \leq \cdots \leq I(f) \leq \cdots \leq V_{2,6}(f) \leq V_{2,4}(f) \leq V_{2,3}(f), \tag{3.5.15}$$

and if $f'''(x) \geq 0$ for all $x \in [a, b]$, then

$$V_{2,3}(f) \leq V_{2,4}(f) \leq V_{2,6}(f) \leq \cdots \leq I(f) \leq \cdots \leq V_{1,6}(f) \leq V_{1,4}(f) \leq V_{1,3}(f), \tag{3.5.16}$$

EXAMPLE 3.5.1. (Schmeisser and Schirmeier 1976) Consider $\int_{-1}^1 e^{-x^2} dx = 2 \int_0^1 e^{-x^2} dx$. Since the third derivative of the integrand is positive on $[0, 1]$, we get the following monotone bounds.

Table 3.5.1

n	$V_{2,n}$	$V_{1,n}$
4	1.4878637	1.4993485
6	1.4929523	1.4943389
10	1.4935622	1.4937340
18	1.4936375	1.4936589
34	1.4936468	1.4936496 ■

Table 3.5.2. Gaussian Quadratures: $\int_a^b w(x) f(x) dx = \sum_{k=1}^n w_k f(x_k) + E_n$.

Weight $w(x)$	Interval (a, b)	Nodes are zeros of	Nodes x_k	Weights w_k	Error Coefficient K_n
1	$(-1, 1)$	$P_n(x)$	See Table A.6	$\frac{-2}{(n+1) P_{n+1}(x_k) P'_n(x_k)}$	$\frac{2^{2n+1} (n!)^4}{(2n+1) [(2n)!]^3}$
e^{-x}	$(0, \infty)$	$L_n(x)$	See Table A.7	$\frac{(n!)^2 x_k}{(n+1)^2 L_{n+1}^2(x_k)}$	$\frac{(n!)^2}{(2n)!}$
e^{-x^2}	$(-\infty, \infty)$	$H_n(x)$	See Table A.8	$\frac{2^{n-1} n! \sqrt{\pi}}{n^2 H_{n-1}^2(x_k)}$	$\frac{(n!) \sqrt{\pi}}{2^n (2n)!}$
$\frac{1}{\sqrt{1-x^2}}$	$(-1, 1)$	$T_n(x)$	$\cos \frac{(2k-1)\pi}{2n}$	$\frac{\pi}{n}$	$\frac{2\pi}{2^{2n} (2n)!}$
$\sqrt{1-x^2}$	$(-1, 1)$	$U_n(x)$	$\cos \frac{k\pi}{n+1}$	$\frac{\pi}{n+1} \sin^2 \frac{k\pi}{n+1}$	$\frac{\pi}{2^{2n+1} (2n)!}$
$\sqrt{\frac{x}{1-x^2}}$	$(0, 1)$	$\frac{T_{2n+1}(\sqrt{x})}{\sqrt{x}}$	$\cos^2 \frac{(2k-1)\pi}{4n+2}$	$\frac{2\pi}{2n+1} \cos^2 \frac{(2k-1)\pi}{4n+2}$	$\frac{\pi}{2^{4n+1} (2n)!}$
$\sqrt{\frac{1-x}{1+x}}$	$(0, 1)$	$P_n^{(1/2, -1/2)}(x)$	$\cos \frac{2k\pi}{2n+1}$	$\frac{4\pi}{2n+1} \sin^2 \frac{k\pi}{2n+1}$	$\frac{\pi}{2^{2n} (2n)!}$
$\frac{1}{\sqrt{x}}$	$(0, 1)$	$P_{2n}(\sqrt{x})$	$(x_k^+)^2$	$2h_k$	$\frac{2^{4n+1} [(2n)!]^3}{(4n+1) [(4n)!]^2}$
\sqrt{x}	$(0, 1)$	$\frac{P_{2n+1}(\sqrt{x})}{\sqrt{x}}$	$(x_k^+)^2$	$2h_k (x_k^+)^2$	$\frac{2^{4n+3} [(2n+1)!]^4}{(4n+3) [(4n+2)!]^2 (2n)!}$

Here, the error $E_n = K_n f^{(2n)}(\xi)$, $a < \xi < b$. Also, x_k^+ denotes the k -th positive zero of $P_{2n}(x)$ or $P_{2n+1}(x)$ of the previous column, and h_k denotes the corresponding weights for x_k^+ in the Gauss-Legendre formula ($w(x) = 1$).

3.6. Gaussian Rules for the Moments

The formula for the Gaussian moments is

$$\int_0^1 x^k f(x) dx = \sum_{i=1}^n w_i f(x_i) + R_n. \quad (3.6.1)$$

3.6.1. Gauss-Jacobi Moments. Formula (3.6.1) yields the Gauss-Jacobi rule, when it is used with the polynomials

$$q_n = \sqrt{k+2n+1} P_n(k, 0)(1-2x),$$

where $P_n(k, 0)(x)$ are the Jacobi polynomials, the quadrature point x_i is the i -th zero of q_n ; the weights are given by $w_i = \left[\sum_{j=0}^{n-1} [q_j(x_i)]^2 \right]^{-1}$, and the remainder is

$$R_n = \left[\frac{n!(k+n)!}{(k+2n)!} \right]^2 \frac{f^{(2n)}(\xi)}{(k+2n+1)(2n)!}, \quad 0 < \xi < 1.$$

The points x_i and weights w_i are available in Abramowitz and Stegun (1968, p. 921). For nodes, see [gaussmoments.nb](#) on the CD-R.

3.6.2. Gauss-Legendre Moments. There are two cases.

CASE 1. The Gaussian rule (3.6.1), when used with the polynomials

$$(1-x)^{-1/2} P_{2n+1}(\sqrt{1-x}), \quad P_{2n+1}(1) = 1,$$

where $P_n(x)$ are the Legendre polynomials, yields the rule

$$\int_0^1 f(x) \sqrt{1-x} dx = \sum_{i=1}^n w_i f(x_i) + R_n,$$

where the quadrature point $x_i = 1 - \xi_i^2$, where ξ_i is the i -th positive zero of $P_{2n+1}(x)$; the weights are given by $w_i = 2\xi_i^2 w_i^{(2n+1)}$, where w_i^{2n+1} are the weights of order $2n+1$, and the remainder is

$$R_n = \frac{2^{4n+3} [(2n+1)!]^4}{(2n)!(4n+3)[(4n+2)!]^2} f^{(2n)}(\xi), \quad 0 < \xi < 1.$$

CASE 2. Using the polynomials $P_{2n}(\sqrt{1-x})$, $P_{2n}(1) = 1$, we have

$$\int_0^1 \frac{f(x)}{\sqrt{1-x}} dx = \sum_{i=0}^n w_i f(x_i) + R_n,$$

where the quadrature points are $x_i = 1 - \xi_i$, ξ_i being the i -th zero of $P_{2n}(x)$; the weight $w_i = 2w_i^{(2n)}$, where $w_i^{(2n)}$ are the weights of order $2n$, and the remainder is

$$R_n = \frac{2^{4n+1} [(2n)!]^3}{(4n+1) [(4n)!]^2} f^{(2n)}(\xi), \quad 0 < \xi < 1.$$

3.6.3. Gauss-Legendre Moments on an Arbitrary Interval. There are two cases.

CASE 1. Formula (3.6.1), when used with the polynomials

$$(1-x)^{-1/2} P_{2n+1}(\sqrt{1-x}), \quad P_{2n+1}(1) = 1,$$

where $P_n(x)$ are the Legendre polynomials, yields the rule

$$\int_a^b f(y) \sqrt{b-y} dx = (b-a)^{3/2} \sum_{i=1}^n w_i f(y_i) + R_n,$$

where the quadrature point $x_i = 1 - \xi_i^2$, ξ_i being the i -th positive zero of $P_{2n+1}(x)$; the weights are given by $w_i = 2\xi_i^2 w_i^{(2n+1)}$, where w_i^{2n+1} are the weights of order $2n+1$, and the remainder is

$$R_n = \frac{(b-a)^{2n+1} 2^{4n+3} [(2n+1)!]^4}{(2n)!(4n+3)[(4n+2)!]^2} f^{(2n)}(\xi), \quad 0 < \xi < 1.$$

CASE 2. Related to the polynomials $P_{2n}(\sqrt{1-x})$, $P_{2n} = 1$, we have

$$\int_a^b \frac{f(y)}{\sqrt{b-y}} dy = \sqrt{b-a} \sum_{i=1}^n w_i f(y_i) + R_n,$$

where $y_i = a + (b-a)x_i$; the point $x_i = 1 - \xi_i^2$, where ξ_i is the i -th zero of $P_{2n}(x)$; the weights are $w_i = 2w_i^{(2n)}$, where $w_i^{(2n)}$ are the weights of order $2n$.

3.6.4. Gauss-Chebyshev Moments. Related to the orthogonal polynomials $\frac{1}{\sqrt{x}} T_{2n+1}(\sqrt{x})$, we have

$$\int_0^1 f(x) \sqrt{\frac{x}{1-x}} dx = \sum_{i=1}^n w_i f(x_i) + R_n,$$

where the quadrature points are $x_i = \cos^2 \frac{(2i-1)\pi}{2(2n+1)}$; the weights are $w_i = \frac{2\pi}{2n+1} x_i$; and the remainder is

$$R_n = \frac{\pi}{(2n)! 2^{4n+1}} f^{(2n)}(\xi), \quad 0 < \xi < 1.$$

3.6.5. Gauss-Chebyshev Moments on an Arbitrary Interval. Related to the orthogonal polynomials $\frac{1}{\sqrt{x}} T_{2n+1}(\sqrt{x})$, we have

$$\int_a^b f(x) \sqrt{\frac{x-a}{b-x}} dx = (b-a) \sum_{i=1}^n w_i f(y_i) + R_n,$$

where the quadrature points are $y_i = a + (b-a)x_i$, with $x_i = \cos^2 \frac{(2i-1)\pi}{2(2n+1)}$; the weights are the same as in §3.2.7.

3.6.6. Weights and Modified Moments. Piessens (1987) has classified the following 18 types of weight functions $w(x)$ and provided the related recurrence relations for the computation of modified moments, which are defined by $M_n = \int_{-1}^1 w(x) T_n(x) dx$, where $T_n(x)$ are the Chebyshev polynomials of the first kind (see Gautschi 1970, and Table 3.6.1 on pages 151–159).

1. $w_1(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$,
2. $w_2(x) = (1-x)^\alpha(1+x)^\beta e^{-ax}$, $\alpha, \beta > -1$,
3. $w_3(x) = (1-x)^\alpha(1+x)^\beta \ln\left(\frac{1+x}{2}\right) e^{-ax}$, $\alpha > -2, \beta > -1$,
4. $w_4(x) = e^{-ax^2}$,
5. $w_5(x) = (1-x)^\alpha(1+x)^\beta e^{-a(x+1)^2}$, $\alpha, \beta > -1$,
6. $w_6(x) = (1-x)^\alpha(1+x)^\beta e^{-a/(x+1)}$, $\alpha, \beta > -1$,
7. $w_7(x) = (1-x)^\alpha(1+x)^\beta e^{-a/x^2}$,
8. $w_8(x) = (1-x)^\alpha(1+x)^\beta e^{-a/(x+1)^2}$, $\alpha, \beta > -1$,
9. $w_9(x) = (1-x)^\alpha(1+x)^\beta \ln\left(\frac{1+x}{2}\right)$, $\alpha, \beta > -1$,
10. $w_{10}(x) = (1-x)^\alpha(1+x)^\beta \ln\left(\frac{1+x}{2}\right) \ln\left(\frac{1-x}{2}\right)$, $\alpha, \beta > -2$,
11. $w_{11}(x) = |x-a|^\alpha$, $\alpha > -1$ and $|a| < 1$, or α arbitrary and $|a| > 1$,
12. $w_{12}(x) = |x-a|^\alpha \operatorname{sgn}(x-a)$, $\alpha > -1$,
13. $w_{13}(x) = |x-a|^\alpha \ln|x-a|$, $\alpha > -1$,
14. $w_{14}(x) = |x-a|^\alpha \ln|x-a| \operatorname{sgn}(x-a)$, $\alpha > -1$,
15. $w_{15}(x) = (1-x)^\alpha(1+x)^\beta |x-a|^\gamma$, $\alpha > -1$,
16. $w_{16}(x) = (1-x)^\alpha(1+x)^\beta |x-a|^\gamma \ln|x-a|$, $\alpha > -1$,
17. $w_{17}(x) = [(x-b)^2 + a^2]^\alpha$, $\alpha > -1$,
18. $w_{18}(x) = (1+x)^\alpha J_\nu(a(x+1)/2)$, $\alpha > -1$,

where a is real or complex. The modified moments are presented in Table 3.6.1.

Table 3.6.1. Table of Modified Moments.

Weight	Modified Moments (RR)	Stability
1. $w_1(x)$	<p>RR is $(\alpha + \beta + n + 2) M_{n+1} + 2(\alpha - \beta) M_n + (\alpha + \beta - n + 2) M_{n-1} = 0$, with $M_0 = 2^{\alpha+\beta+1} B(\alpha + 1, \beta + 1)$, $M_1 = \frac{\beta - \alpha}{\alpha + \beta + 2} M_0$. Explicit: $M_n = 2^{\alpha+\beta+1} \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} {}_3F_2\left[\begin{matrix} n, -n, \alpha + 1 \\ \frac{1}{2}, \alpha + \beta + 2 \end{matrix}; 1\right]$. $M_n \sim \sum_{k=0}^{\infty} a_k(\alpha, \beta) c(\alpha + k) n^{-2(\alpha+k+1)}$ $+ (-1)^n \sum_{k=0}^{\infty} a_k(\beta, \alpha) c(\beta + k) n^{-2(\beta+k+1)}$, $c(\alpha) = \cos((\alpha + 1)\pi) \Gamma(2\alpha + 2)$, $a_0(\alpha, \beta) = 2^{\beta-\alpha}$, $a_1(\alpha, \beta) = -\frac{\alpha + 2\beta + 2}{3} 2^{\beta-\alpha-2}$, $a_2(\alpha, \beta) = \left(\frac{4}{15} + \frac{19\alpha}{45} + \frac{\alpha^2}{9} + \frac{2\alpha\beta}{3} + \beta + \beta^2\right) 2^{\beta-\alpha-5}$. For $\alpha = \beta$: RR is of order 1. For $\alpha = 0$: RR is $(n - 1)(n + \beta + 1) M_n + n(n - \beta - 2) M_{n-1} = -2^{\beta+1}$.</p>	<p>FR stable for $\alpha < \beta$ and $\alpha \neq \frac{1}{2} + \text{integer}$, or $\alpha > \beta$ and $\beta \neq \frac{1}{2} + \text{integer}$.</p> <p>FR is stable.</p>
2. $w_2(x)$	<p>RR is $\frac{a}{2} M_{n+2} - (n + \alpha + \beta + 2) M_{n+1} - (2\alpha - 2\beta + a) M_n$ $+ (n - \alpha - \beta - 2) M_{n-1} + \frac{a}{2} M_{n-2} = 0$.</p>	

Continued over next 8 pages.

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
	<p>For $\alpha = 0$: RR is $-a M_{n+1} + (2\beta + 2n + 2 - \frac{(n-2)a}{n-1}) M_n$ $+ \left(2\alpha - \beta - 1 - \frac{(\beta + 1 - a)(n+1)}{n-1} \right) M_{n-1} + \frac{an}{n-1} M_{n-2}$ $= -\frac{2^{\beta+2} e^{-1}}{n-1};$ $M_0 = q_1, M_1 = q_2 - q_1, M_2 = 2q_3 - 4q_2 + f_1,$ where $q_n = e^{-a} \Gamma(\alpha + n) P(\alpha + n, 2a) a^{-\alpha-n}.$</p> <p>For $\alpha = \beta = 0$: RR is $\frac{a}{n+1} M_{n+1} - 2M_n - \frac{a}{n-1} M_{n-1} = \frac{2}{n^2-1} [e^{-a} + (-1)^n e^a].$</p> <p>For $\alpha = i\omega$, where ω is real, RR for $M_n = \int_{-1}^1 \cos(\omega x) T_n(x) dx$ is: $\omega^2(n-1)(n-2) M_{n+2} - 2(n^2-4)(\omega^2-2n^2+2) M_n$ $+ \omega^2(n+1)(n-2) M_{n-2} = 24\omega \sin \omega - 8(n^2-4) \cos \omega;$ and RR for $M_n = \int_{-1}^1 \sin(\omega x) T_n(x) dx$ is: $\omega^2(n-1)(n-2) M_{n+2} - 2(n^2-4)(\omega^2-2n^2+2) M_n$ $+ \omega^2(n+1)(n-2) M_{n-2} = -24\omega \cos \omega - 8(n^2-4) \sin \omega.$</p>	<p>FR and BR unstable, Lozier's algorithm needed, see §3.6.7.</p> <p>Lozier's algorithm needed.</p> <p>Lozier's algorithm needed.</p>
3. $w_3(x)$	<p>RR is $\frac{a}{2} M_{n+2} - (n + \alpha + \beta + 2) M_{n+1} - (2\alpha - 2\beta + a) M_n$ $+ (n - \alpha - \beta - 2) M_{n-1} + \frac{a}{2} M_{n-2} = I_{n+1} - 2I_n + I_{n-1},$ where $I_n = \int_{-1}^1 w_2(x) T_n(x) dx.$ $M_n \sim e^{-a} [-2^{\alpha-\beta-2} c(\beta+1) n^{-2\beta-4} + \dots]$ $+ (-1)^n e^a [2^{\beta-\alpha+1} c(\alpha) P_n(\alpha) n^{-2\alpha-2} + \dots],$ where $c(\alpha) = \cos((\alpha+1)\pi) \Gamma(2\alpha+2), P_n(\alpha) = \psi(2\alpha+2) - \ln(2n) - \frac{\pi}{2} \tan(\pi\alpha).$</p>	

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
4. $w_4(x)$	RR is $a(n-1)M_{n+2} + 2(1-n^2-a)M_n - a(n+1)M_{n-2} = 4e^{-a}$, where $M_n = 0$ for odd n , and $M_0 = \sqrt{\pi/a} \operatorname{erf}(\sqrt{a})$. $M_n \sim e^{-a} [2n^{-2} + 2(6a-1)n^{-4} - 2(60a^2-60a+1)n^{-6} + \dots]$.	FR unstable, Use Lozier's algorithm.
5. $w_5(x)$	RR is $aM_{n+3} + 2aM_{n+2} - [a + 2(\alpha + \beta + 2 + n)]M_{n+1} - 4(a + \alpha - \beta)M_n$ $- [a + 2(\alpha + \beta + 2 - n)]M_{n-1} + 2aM_{n-2} + aM_{n-3} = 0$. For $\alpha = 0$, the order of RR is reduced; we have $M_0 = 2^{\alpha+\beta+1} {}_2F_2 \left[\frac{\beta+1}{2}, \frac{\beta+2}{2}, \frac{\alpha+\beta+2}{2}, \frac{\alpha+\beta+3}{2}; -4a \right]$.	
6. $w_6(x)$	RR is $(\alpha + \beta + 3 + n)M_{n+2} + 2(a + 2\alpha + 2 + n)M_{n+1} + 2(3\alpha - \beta - 2a + 1)M_n$ $+ 2(a + 2\alpha + 2 - n)M_{n-1} + (\alpha + \beta + 3 - n)M_{n-2} = 0$; $M_0(\alpha, \beta, a) = 2^{\alpha+\beta+1} e^{-a/2} \Gamma(\alpha+1) U(\alpha+1, -\beta, a/2)$, $M_1(\alpha, \beta, a) = -M_0(\alpha+1, \beta, a) + M_0(\alpha, \beta, a)$, $M_2(\alpha, \beta, a) = \frac{(\beta - 3\alpha + 2a - 1)M_0(\alpha, \beta, a) - 2(2\alpha + a + 2)M_1(\alpha, \beta, a)}{\alpha + \beta + 3}$.	FR and BR unstable, use Lozier's algorithm.
7. $w_7(x)$	RR is $(\alpha + \beta + 5 + n)M_{n+4} + 2(\alpha - \beta)M_{n+3}$ $+ [4(\alpha + \beta + 2 + 2a) + 2n]M_{n+2} + 6(\alpha - \beta)M_{n+1}$ $+ [6(\alpha + \beta + 1) - 16a]M_n + 6(\alpha - \beta)M_{n-1}$ $+ [4(\alpha + \beta + 2 + 2a) - 2n]M_{n-2} + 2(\alpha - \beta)M_{n-3} + 6(\alpha - \beta)M_{n-1}$ $+ (\alpha + \beta + 5 - n)M_{n-4} = 0$.	

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
8. $w_8(x)$	RR is $(\alpha + \beta + 4 + n) M_{n+3} + 2(3\alpha - \beta + 6 + 2n) M_{n+2}$ $+ (15\alpha - \beta + 12 + 8a + 5n) M_{n+1} + 4(5\alpha - \beta + 2 - 4a) M_n$ $+ (15\alpha - \beta + 8a - 5n) M_{n-1} + 2(3\alpha + \beta + 6 + 2n) M_{n-2}$ $+ (\alpha + \beta + 4 - n) M_{n-3} = 0.$	
9. $w_9(x)$	RR is $(\alpha + \beta + n + 2) M_{n+1} + 2(\alpha - \beta) M_n + (\alpha + \beta - n + 2) M_{n-1}$ $= 2I_n - I_{n+1} - I_{n-1},$ where $I_n = \int_{-1}^1 (1-x)^\alpha (1+x)^\beta T_n(x) dx.$	
10. $w_{10}(x)$	RR is $(\alpha + \beta + n + 2) M_{n+1} + 2(\alpha - \beta) M_n + (\alpha + \beta - n + 2) M_{n-1}$ $= 2H_n - H_{n+1} - H_{n-1} - 2G_n - G_{n+1} - G_{n-1},$ where $H_n = \int_{-1}^1 (1-x)^\alpha (1+x)^\beta \ln\left(\frac{1-x}{2}\right) T_n(x) dx,$ and $G_n = \int_{-1}^1 (1-x)^\alpha (1+x)^\beta \ln\left(\frac{1+x}{2}\right) T_n(x) dx.$ $M_n \sim A_n(\alpha, \beta) + (-1)^n A_n(\beta, \alpha),$ where $A_n(\alpha, \beta) = 2^{\beta-\alpha-1} C(\alpha+1) P_n(\alpha+1) n^{-2\alpha-4}$ $- \frac{2^{\beta-\alpha-4}}{3} C(\alpha+2) [(2\alpha+6\beta+3) P_n(\alpha+2) + 1] n^{-2\alpha-6} + \dots,$ $C(\alpha) = \cos(\pi\alpha) \Gamma(2\alpha+2), P_n(\alpha) = \psi(2\alpha+2) - \ln 2n - \frac{\pi}{2} \tan(\pi\alpha);$ $M_0 = 2^{\alpha+\beta+1} B(\alpha+1, \beta+1) [(\psi(\alpha+1) - \psi(\alpha+\beta+2))$ $- (\psi(\beta+1) - \psi(\alpha+\beta+2) - \psi'(\alpha+\beta+2))],$ $M_1 = M_0(\alpha, \beta+1) - M_0(\alpha, \beta).$ where $\psi(x)$ is the psi function and $B(x, y)$ the beta function.	FR stable

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
11. $w_{11}(x)$	<p>RR is $\left(1 + \frac{\alpha + 1}{n + 1}\right) M_{n+1} - 2a M_n + \left(1 - \frac{\alpha + 1}{n + 1}\right) M_{n-1}$</p> <p>$= \frac{2}{1 - n^2} [(1 - a)^{\alpha+1} - (-1)^n (1 + a)^{\alpha+1}].$</p> <p>For $a < 1$ and $\alpha > -1$, we have</p> <p>$M_n \sim \sum_{k=0}^{\infty} (-1)^{k+1} (2k + 1)! [r_k(a) + (-1)^n r_k(-a)] n^{-2k-2}$</p> <p>$+ 2 \sum_{k=0}^{\infty} s_{2k} \cos(n \arccos a) \cos((\alpha + 2k + 1)\pi/2) \Gamma(\alpha + 2k + 1) n^{-\alpha-2k-1}$</p> <p>$- 2 \sum_{k=0}^{\infty} s_{2k+1} \sin(n \arccos a) \sin((\alpha + 2k + 2)\pi/2) \Gamma(\alpha + 2k + 2) n^{-\alpha-2k-2},$</p> <p>where $r_0 = (1 - a)^\alpha$, $r_1 = -\left(\frac{(1 - a)^\alpha}{3!} + \frac{\alpha(1 - a)^{\alpha-1}}{2}\right)$,</p> <p>$s_0 = (1 - a^2)^{(\alpha+1)/2}$, $s_1 = a\left(1 - \frac{\alpha}{2}\right) (1 - a^2)^{\alpha/2}$;</p> <p>$M_0 = \frac{1}{\alpha + 1} [(1 - a)^{\alpha+1} + (1 + a)^{\alpha+1}],$</p> <p>$M_1 = \frac{1}{\alpha + 2} [(1 - a)^{\alpha+2} + (1 + a)^{\alpha+2}] + a M_0,$</p> <p>$M_2 = \frac{2}{\alpha + 3} [(1 - a)^{\alpha+3} + (1 + a)^{\alpha+3}] + 4a M_1 - (2a^2 + 1) M_0.$</p>	FR stable

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
12. $w_{12}(x)$	<p>RR is the same as for $w_{11}(x)$. For $a < 1$ and $\alpha > -1$, we have</p> $M_n \sim \sum_{k=0}^{\infty} (-1)^{k+1} (2k+1)! [r_k(a) + (-1)^n r_k(-a)] n^{-2k-2}$ $+ 2 \sum_{k=0}^{\infty} s_{2k} \sin(n \arccos a) \sin((\alpha + 2k + 1)\pi/2) \Gamma(\alpha + 2k + 1) n^{-\alpha-2k-1}$ $- 2 \sum_{k=0}^{\infty} s_{2k+1} \cos(n \arccos a) \cos((\alpha + 2k + 2)\pi/2) \Gamma(\alpha + 2k + 2) n^{-\alpha-2k-2},$ <p>where r_k and s_k are the same as in $w_{11}(x)$; and</p> $M_0 = \frac{1}{\alpha+1} [(1-a)^{\alpha+1} - (1+a)^{\alpha+1}],$ $M_1 = \frac{1}{\alpha+2} [(1-a)^{\alpha+2} - (1+a)^{\alpha+2}] + a M_0,$ $M_2 = \frac{2}{\alpha+3} [(1-a)^{\alpha+3} - (1+a)^{\alpha+3}] + 4a M_1 - (2a^2 + 1) M_0.$	
13. $w_{13}(x)$	<p>RR is $(n-1)(n+\alpha+2) M_{n+1} - 2a(n^2-1) M_n + (n+1)(n-\alpha-2) M_{n-1}$ $= 2(-1)^n (a+1)^{\alpha+1} \ln(1+a) - 2(1-a)^{\alpha+1} \ln(1-a)$ $-(n-1) I_{n+1} + (n+1) I_{n-1}$, where $I_n = \int_{-1}^1 x-a ^\alpha T_n(x) dx$; $M_0 = P(\alpha, a) + P(\alpha, -a)$, $M_1 = aP(\alpha, a) + aP(\alpha, -a) + P(\alpha+1, -a) - P(\alpha+1, a)$, $M_2 = 2P(\alpha+2, a) + 2P(\alpha+2, -a) + (2a^2-1) [P(\alpha, a) + P(\alpha, -a)]$ $+ 4a [P(\alpha+1, -a) - P(\alpha+1, a)]$, where $P(\alpha, a) = \frac{(1+a)^{\alpha+1}}{\alpha+1} \ln(1+a) - \frac{(1+a)^{\alpha+1}}{(\alpha+1)^2}$.</p>	FR stable for $ a < 1$.

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
14. $w_{14}(x)$	RR is $(n-1)(n+\alpha+2) M_{n+1} - 2a(n^2-1) M_n + (n+1)(n-\alpha-2) M_{n-1}$ $= (n+1) I_{n-1} - (n-1) I_{n+1}$ $-2(1-a)^{\alpha+1} \ln(1-a) - 2(1+a)^{\alpha+1} \ln(1+a),$ where $I_n = \int_{-1}^1 x-a ^\alpha \operatorname{sgn}(x-a) T_n(x) dx,$ and the starting values are similar to those for $w_{13}(x)$.	FR stable.
15. $w_{15}(x)$	RR is $(\alpha+\beta+\gamma+3+n) M_{n+2} + 2[(1-a)(\alpha+1) - (1+a)(\beta+1) - an] M_{n+1}$ $+2[(1-2a)(\alpha+1) + (1+2a)(\beta+1) - (\gamma+1)] M_n$ $+2[(1-a)(\alpha+1) - (1+a)(\beta+1) + an] M_{n-1}$ $+(\alpha+\beta+\gamma+3-n) M_{n-2} = 0;$ $M_0 = J(\alpha, \beta, \gamma, a) + J(\beta, \alpha, \gamma, -a),$ $M_1 = a M_0 + J(\gamma+1, \beta, \alpha, -a) - J(\gamma+1, \alpha, \beta, a),$ $M_2 = \frac{1}{\alpha+\beta+\gamma+3} \{2[(1-a)(\beta+1) - (1-a)(\alpha+1)] M_1$ $[(\gamma+1) - (1-2a)(\alpha+1) - (1+2a)(\beta+1)] M_0\},$ where $J(\alpha, \beta, \gamma, a)$ $= 2^\alpha(1+a)^{\beta+\gamma+1} B(\beta+1, \gamma+1) {}_2F_1(-\alpha, \beta+1; \gamma+\beta+2; (1+a)/2).$	FR stable.

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
16. $w_{16}(x)$	RR is $(\alpha + \beta + \gamma + 3 + n) M_{n+2} + 2 [(1 - a)(\alpha + 1) - (1 + a)(\beta + 1) - an] M_{n+1}$ $+ 2 [(1 - 2a)(\alpha + 1) + (1 + 2a)(\beta + 1) - (\gamma + 1)] M_n$ $+ 2 [(1 - a)(\alpha + 1) - (1 + a)(\beta + 1) + an] M_{n-1} + (\alpha + \beta + \gamma + 3 - n) M_{n-2}$ $= 2I_n - I_{n+2} - I_{n-2}$, where $I_n = \int_{-1}^1 (1 - x)^\alpha (1 + x)^\beta x - a ^\gamma T_n(x) dx$.	FR stable.
17. $w_{17}(x)$	RR is $\left(\frac{1}{4} + \frac{\alpha + 1}{2(n + 1)}\right) M_{n+2} - b\left(1 + \frac{\alpha + 1}{n + 1}\right) M_{n+1}$ $+ \left(a^2 + b^2 + \frac{1}{2} + \frac{\alpha + 1}{1 - n^2}\right) M_n - b\left(1 + \frac{\alpha + 1}{1 - n}\right) M_{n-1}$ $+ \left(\frac{1}{4} + \frac{\alpha + 1}{2(1 - n)}\right) M_{n-2} = \frac{(a^2 + (1 - b)^2)^{\alpha+1} + (-1)^n (a^2 + (1 + b)^2)^{\alpha+1}}{1 - n^2}$. For $\alpha = -1$, $M_0 = \frac{1}{a} \left(\arctan \frac{1 - b}{a} + \arctan \frac{1 + b}{a} \right)$, $M_1 = b M_0 + \frac{1}{2} \ln \frac{a^2 + (1 - b)^2}{a^2 + (1 + b)^2}$, $M_2 = 4b M_1 - (2a^2 + 2b^2 + 1) M_0 + 4$. For $b = 0$, we have $M_0 = \begin{cases} -2 \ln \frac{ \alpha }{1 + \sqrt{1 + a^2}} & \text{if } \alpha = -\frac{1}{2}, \\ \frac{2}{\alpha} \arctan \frac{1}{a} & \text{if } \alpha = -1, \end{cases}$ $(1 + 2\alpha) M_1(\alpha) = 2(1 + a^2)^\alpha + 2\alpha a^2 M_0(\alpha - 1)$, $(3 + 2\alpha) M_2(\alpha) = 4(1 + a^2)^\alpha - (3 + 2\alpha + 2a^2) M_0(\alpha)$.	FR unstable

Table 3.6.1. Table of Modified Moments, Continued.

Weight	Modified Moments (RR)	Stability
18. $w_{18}(x)$	RR is $\frac{\omega}{16} M_{n+4} + [(n+3)(n+3+2\alpha) + \alpha^2 - \nu^2 - \omega^2/4] M_{n+2}$ $+ [4(\nu^2 - \alpha^2) - 2(n+2)(2\alpha-1)] M_{n+1}$ $- [2(n^2 - 4) + 6(\nu^2 - \alpha^2) - 2(2\alpha-1) - 3\omega^2/8] M_n$ $+ [4(\nu^2 - \alpha^2) + 2(n-2)(2\alpha-1)] M_{n-1}$ $+ [(n-3)(n-3-2\alpha) + (\alpha^2 - \nu^2 - \omega^2/4)] M_{n-2} + \frac{\omega^2}{16} M_{n-4} = 0,$ where $M_0 = G(\omega, \nu, \alpha)$, $M_1 = 2G(\omega, \nu, \alpha+2) - G(\omega, \nu, \alpha)$, $M_2 = 8G(\omega, \nu, \alpha+2) - 8G(\omega, \nu, \alpha+1) + G(\omega, \nu, \alpha)$, $M_3 = 32G(\omega, \nu, \alpha+3) - 48G(\omega, \nu, \alpha+2)$ $+ 18G(\omega, \nu, \alpha+1) - G(\omega, \nu, \alpha)$, where $G(\omega, \nu, \alpha) = \int_0^1 x^\alpha J_\nu(\omega x) dx$. $M_n \sim -\frac{1}{2} J_n(\omega) n^{-2}$ $+ (-1)^n 2^{-3\nu-2\alpha-1} \frac{\omega^\nu}{\Gamma(\nu+1)} \cos((\alpha+1)\pi) \Gamma(2\alpha+2) n^{-2\alpha-2\nu-2}.$	FR stable for very large $ a $. For small $ a $ use Lozier's algorithm, with 6 initial values and 2 end values.

- NOTES. 1. If we set $f_n = {}_3F_2 \left[\begin{matrix} n, -n, \alpha+1 \\ \frac{1}{2}, \alpha+\beta+2 \end{matrix}; 1 \right]$, then, using Fesenmeyer's technique (see Rainville 1960), we obtain the recurrence relation $(\alpha+\beta+n+2) f_{n+1} + 2(\alpha-\beta) f_n + (\alpha+\beta-n+2) f_{n-1} = 0$, which yields $f_0 = 1$, $f_1 = \frac{\beta-\alpha}{\alpha+\beta+2}$, $f_2 = \frac{2(\alpha-\beta)^2}{(\alpha+\beta+2)(\alpha+\beta+3)} - \frac{(\alpha+\beta+1)}{(\alpha+\beta+2)}$, \dots
2. In $w_6(x)$, page 156, $U(\alpha, \beta, a)$ and $M_0(\alpha, \beta, a)$ are Kummer's confluent hypergeometric functions.

These modified moments are presented by their respective recurrence relations (RR's) for the types of weight functions $w_1(x)$ through $_{18}(x)$; under 'stability' it is noted whether the forward recursion (FR) or the backward recursion (BR) is stable; and asymptotic expansions of M_n as $n \rightarrow \infty$ are given.

NOTES: (i) The modified moments for $w_1(x)$ are useful in computing integrals of the type $\int_a^b (b-x)^\alpha (x-a)^\beta f(x) dx$ which have algebraic endpoint singularities (Piessens and Branders 1973, and Piessens, Mertens and Branders 1974).

(ii) The modified moments for $w_2(x)$ for $a = i\omega$ are useful in computing the Fourier coefficients $\int_a^b \cos(\omega x) dx$ (Piessens and Branders 1975), and for constructing the Gaussian quadrature formulas for $\int_0^1 \left(1 + \left\{ \frac{\cos(\omega x)}{\sin(\omega x)} \right\} \right) f(x) dx$.

(iii) The starting values for the modified moments of $w_7(x)$ and $w_8(x)$ are not yet known and further study is needed.

(iv) Stating values and applications of $w_9(x)$ are available in Piessens and Branders (1973).

(v) The computation of integrals in the modified moments for $w_{18}(x)$ is available in Luke (1962).

3.6.7. Lozier's Algorithm. (Lozier 1980) This algorithm concerns the problem of computing solutions to recurrence relations of second and higher orders. For a numerical solution to be stable, it is necessary to determine the relative rates of growth that can be exhibited by solutions, and to set boundary conditions accordingly. Details and some examples can be found in Lozier (1980) and Wimp (1984).

3.6.8. Values of the Moments M_n for the Weight Function $w_1(x)$. The following table gives the exact values of $M_n(\alpha, \beta)$ for $\alpha = 1.1$ and $\beta = -0.4$ (Piessens and Branders 1973). The relative in the third column is in single precision computation.

n	Values of $M_n(1.1, -0.4)$	Relative Error
0	3.27778944(0)	4.0(-7)
10	-5.1022612(-2)	3.1(-6)
20	-2.2090810(-2)	4.0(-6)
50	-7.3428042(-3)	1.3(-5)
100	-3.1951796(-3)	2.7(-5)
200	-1.3906742(-3)	4.5(-5)
300	-8.5488856(-4)	7.2(-5)

3.7. Finite Oscillatory Integrals

The transformation $x = \frac{b-a}{2}y + \frac{b+a}{2} = my + c$ reduces the integral $I_a^b(wf)$ to

$$m \int_{-1}^1 w(my + c) f(my + c) dy. \quad (3.7.1)$$

For $w(x) = \sin(tx)$ or $w(x) = \cos(tx)$, we have

$$w(my + c) = \begin{cases} \cos(mty) \cos(ct) - \sin(mty) \sin(ct), \\ \sin(mty) \cos(ct) + \cos(mty) \sin(ct), \end{cases} \quad (3.7.2)$$

which yields in each case two integrals of the type

$$K \int_{-1}^1 \begin{cases} \cos \\ \sin \end{cases} (Ty) F(y) dy, \quad (3.7.3)$$

where K is either $\sin(ct)$ or $\cos(ct)$, $T = tm$, and $F(y) = f(my + c)$.

3.7.1. Filon's Formulas for Trigonometric Functions. Let $a = x_0 < x_1 < \dots < x_{2n} = b$, and $f_k = f(x_k)$. There are two formulas:

$$\begin{aligned} \int_{x_0}^{x_{2n}} f(x) \sin(tx) dx &\approx h \left[\alpha(\theta) \{ f_0 \cos(tx_0) - f_{2n} \sin(tx_{2n}) \} \right. \\ &\quad \left. + \beta(\theta) S_{2n} + \gamma(\theta) S_{2n-1} + \frac{2}{45} th^4 C'_{2n-1} \right] - R_n, \end{aligned} \quad (3.7.4)$$

$$\begin{aligned} \int_{x_0}^{x_{2n}} f(x) \cos(tx) dx &\approx h \left[\alpha(\theta) \{ f_{2n} \cos(tx_{2n}) - f_0 \sin(tx_0) \} \right. \\ &\quad \left. + \beta(\theta) C_{2n} + \gamma(\theta) C_{2n-1} + \frac{2}{45} th^4 S'_{2n-1} \right] - R_n, \end{aligned} \quad (3.7.5)$$

where $\theta = th$, and

$$\begin{aligned} S_{2n} &= \sum_{k=0}^n f_{2k} \sin(tx_{2k}) - \frac{1}{2} [f_{2n} \sin(tx_{2n}) + f_0 \sin(tx_0)], \\ S_{2n-1} &= \sum_{k=1}^n f_{2k-1} \sin(tx_{2k-1}), \\ C_{2n} &= \sum_{k=0}^n f_{2k} \cos(tx_{2k}) - \frac{1}{2} [f_{2n} \cos(tx_{2n}) + f_0 \cos(tx_0)], \end{aligned}$$

$$C_{2n-1} = \sum_{k=1}^n f_{2k-1} \cos(tx_{2k-1}),$$

$$S'_{2n-1} = \sum_{k=1}^n f_{2k-1}^{(3)} \sin(tx_{2k-1}),$$

$$C'_{2n-1} = \sum_{k=1}^n f_{2k-1}^{(3)} \cos(tx_{2k-1})$$

$$R_n = \frac{1}{90} nh^5 f^{(4)}(\xi) + O(th^7),$$

$$\alpha(\theta) = \frac{1}{\theta} + \frac{\sin 2\theta}{2\theta^2} - \frac{2\sin^2 \theta}{\theta^3},$$

$$\beta(\theta) = 2\left(\frac{1 + \cos^2 \theta}{\theta^2} - \frac{\sin 2\theta}{\theta^3}\right),$$

$$\gamma(\theta) = 4\left(\frac{\sin \theta}{\theta^3} - \frac{\cos \theta}{\theta^2}\right).$$

For small θ , we have

$$\begin{aligned}\alpha &= \frac{2\theta^3}{45} - \frac{2\theta^5}{315} + \frac{2\theta^7}{4725} + \dots, \\ \beta &= \frac{2}{3} + \frac{2\theta^2}{15} - \frac{4\theta^4}{105} + \frac{2\theta^6}{567} - \dots, \\ \gamma &= \frac{4}{3} - \frac{2\theta^2}{15} + \frac{\theta^4}{210} - \frac{\theta^6}{11340} + \dots\end{aligned}$$

If $f(x)$ is approximated linearly in each subinterval, we have an equivalent form (due to Clendenin 1966)

$$\int_{x_0}^{x_{2n}} f(x) \sin tx \, dx = S_1 + S_2, \quad (3.7.6)$$

where

$$S_1 = y \sum_{k=1}^{n-1} f_{2k} \sin tx_{2k},$$

$$S_2 = f_0 \left[\frac{\cos(tx_0)}{t} - z \cos t(x_0 + h/2) \right] + f_{2n} \left[-\frac{\cos(tx_{2n})}{t} + z \cos t(x_0 + h/2) \right],$$

$$y = \frac{4}{ht^2} \sin^2\left(\frac{th}{2}\right), \quad z = \frac{2}{ht^2} \sin\left(\frac{th}{2}\right), \quad x_k = x_0 + kh.$$

Note that we can use the Lagrangian representation to generate the formula for $I_a^b(f)$, that is

$$I_a^b(f) \approx \int_a^b \sum_{j=0}^n l_j(x) f(x_j) \, dx + E_n = \sum_{j=0}^n C_{n,j} f(x_j) + E_n, \quad (3.7.7)$$

where

$$\begin{aligned} C_{n,j} &= \int_a^b l_j(x) dx = \int_a^b \frac{(x-x_0) \dots (x-x_{j-1})(x-x_{j+1}) \dots (x-x_n)}{(x_j-x_0) \dots (x_j-x_{j-1})(x_j-x_{j+1}) \dots (x_j-x_n)} dx \\ &= \frac{1}{X_{n,j}} \sum_{k=0}^n (-1)^{n-k} \frac{b^{k+1} - a^{k+1}}{k+1} \sigma(j, n, n-k), \end{aligned} \quad (3.7.8)$$

where $X_{n,j} = (x_j - x_0) \dots (x_j - x_{j-1})(x_j - x_{j+1}) \dots (x_j - x_n)$, and the expression $\sigma(j, n, n-k)$ denotes the sum of all possible different products of n quantities x_0, x_1, \dots, x_n taken $(n-k)$ at a time. Applying formula (3.7.7)-(3.7.8) to $\int_a^b f(x) \cos(tx) dx$ and $\int_a^b f(x) \sin(tx) dx$, we find that

$$\begin{aligned} \int_a^b f(x) \cos(tx) dx &\approx \cos t(a+ih) \int_0^h f(a+ih+\xi) \cos(t\xi) d\xi \\ &\quad - \sin t(a+ih) \int_0^h f(a+ih+\xi) \sin(t\xi) d\xi \\ &= \cos t(a+ih) \sum_{j=0}^n C_{n,j}^{\cos} f(a+ih+\xi_j) \\ &\quad - \sin t(a+ih) \sum_{j=0}^n C_{n,j}^{\sin} f(a+ih+\xi_j), \end{aligned} \quad (3.7.9)$$

$$\begin{aligned} \int_a^b f(x) \sin(tx) dx &\approx \sin t(a+ih) \sum_{j=0}^n C_{n,j}^{\cos} f(a+ih+\xi_j) \\ &\quad - \cos t(a+ih) \sum_{j=0}^n C_{n,j}^{\sin} f(a+ih+\xi_j), \end{aligned} \quad (3.7.10)$$

where $h = (b-a)/(n+1)$, $x = a+ih+\xi$, $\xi_j = jh/n$, and

$$\begin{aligned} C_{j,n}^{\cos} &= \frac{1}{T_{n,j}} \sum_{k=0}^n (-1)^{n-k} k! \sigma(j, n, n-k) \\ &\quad \left[\sum_{p=0}^k \frac{\xi^{k-p}}{(k-p)! t^{p+1}} \sin(t\xi + p\pi/2) \right]_0^h, \end{aligned} \quad (3.7.10)$$

$$\begin{aligned} C_{j,n}^{\sin} &= \frac{1}{T_{n,j}} \sum_{k=0}^n (-1)^{n-k} k! \sigma(j, n, n-k) \\ &\quad \left[\sum_{p=0}^k \frac{\xi^{k-p}}{(k-p)! t^{p+1}} \cos(t\xi + p\pi/2) \right]_0^h, \end{aligned} \quad (3.7.11)$$

$$T_{n,j} = (\xi_j - \xi_0) \dots (\xi_j - \xi_{j-1})(\xi_j - \xi_{j+1}) \dots (\xi_j - \xi_n). \quad (3.7.12)$$

The coefficients for the Filon’s quadrature rule are given in Table A.15 for $\theta = 0.0(0.01)0.1(01)1.0$.

EXAMPLE 3.7.1. Compute $I = \int_0^1 e^x \cos tx \, dx$ for $t = 1, 10, 100, 1000, 10000$ and $n \leq 10$; this has the exact value $\frac{e(\cos t + t \sin t)}{1 + t^2}$. The results are given in Table 3.7.1, which shows slow convergence and the loss of accuracy for higher values of t).

Table 3.7.1.

t	Approximate Value	Exact Value
1	1.87802	1.37802
10	-1.68999(-1)	-1.789(-1)
100	-1.35287(-2)	-1.36287(-2)
1000	2.24922(-3)	2.24822(-3)
10000	-8.31005(-5)	-1.83282(-3)

3.7.2. Use of Chebyshev Polynomials and Bessel Functions. If we fit $f(x)$ by a series of Legendre polynomials, then we can obtain formulas for integrals of the form $\int_{-1}^1 T_k(x) \sin(tx) \, dx$ or $\int_{-1}^1 T_k(x) \cos(tx) \, dx$, as suggested by Bakhvalov and Vasileva (1968). Thus,

$$f(x) = \sum_{k=0}^n c_k P_k(x), \quad c_k = \frac{2k+1}{2} \int_{-1}^1 P_k(x) f(x) \, dx. \tag{3.7.13}$$

Then for the oscillatory integrands we have the formula

$$\int_{-1}^1 e^{itx} P_k(x) \, dx = i^k \sqrt{\frac{2\pi}{t}} J_{k+1/2}(t), \tag{3.7.14}$$

and the integral for c_k in (3.7.13) is found by using a $(n+1)$ -point Gauss-Legendre rule which is exact if f is a polynomial of degree $\leq n$. Bakhvalov and Vasileva (1968) also give the recurrence relation

$$I_{n+2} = \left(\frac{2n+4}{t}\right) I_{n+1} - 2I_n + \left(\frac{2n-4}{t}\right) I_{n-1} - I_{n-2}.$$

Alternatively, if $f(x)$ is expanded in terms of Chebyshev polynomials $T_n(x)$ by

$$f(x) = \sum_{k=0}^n a_k T_k(x), \tag{3.7.15}$$

where $a_k = \frac{2}{\pi} \int_{-1}^1 \frac{T_k(x) f(x)}{\sqrt{1-x^2}} dx$ is computed by a Gauss-Chebyshev rule, then we get the formula

$$\int_{-1}^1 f(x) \begin{cases} \cos \\ \sin \end{cases} (tx) dx = \sum_{i=0}^n{}' a_i N_i(t), \quad (3.7.16)$$

where

$$N_k(t) = \int_{-1}^1 T_k(x) e^{itx} dx.$$

Formula (3.7.16) can be regarded as a Lagrangian interpolation polynomial of degree n which collates with $f(x)$ at the $(n+1)$ points $x_j, j = 0, 1, \dots, n$. If these points are taken as the zeros of $T_{k+1}(x)$, i.e., $x_j = \cos \frac{(2j+1)\pi}{2(n+1)}$, then using the orthogonality property of the Chebyshev polynomials, we find that

$$a_i = \frac{2}{n+1} \sum_{j=0}^n f(x_j) \cos \frac{(2j+1)\pi}{2(n+1)}. \quad (3.7.17)$$

An alternative formula to compute a_i is

$$a_i = \frac{2}{\pi} \int_{-1}^1 \frac{T_i(x) f(x)}{\sqrt{1-x^2}} dx. \quad (3.7.18)$$

If $f \in \mathcal{P}_n$, then the integral in (3.7.18) is obtained exactly by using the Gauss-Chebyshev equal weight quadrature rule of order $(n+1)$ with the weight function $w(x) = (1-x^2)^{-1/2}$ on the interval $[-1, 1]$; i.e., we use the general formula

$$\int_{-1}^1 \frac{F(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{n+1} \sum_{j=0}^n F(x_j) + e_{n+1}, \quad (3.7.19)$$

where x_j are given by (3.2.11) and the error term by

$$e_n = \frac{2\pi F^{2n+2}(\theta)}{2^{2n+2} (2n+2)!}, \quad -1 < \theta < 1. \quad (3.7.20)$$

Piessens and Poleunis (1971) use the expansion of e^{itx} in the form

$$e^{itx} = 2 \sum_{j=0}^n{}' i^j J_j(t) T_j(x), \quad (3.7.21)$$

and obtain the formula

$$i^n I_n = -2 \sum_{j=0}^{\infty}{}' i^j J_j(t) \left[\frac{1}{(n+j)^2 - 1} + \frac{1}{(n-j)^2 - 1} \right], \quad (3.7.22)$$

which depends on t , and thus we have an increased amount of computation as t increases.

Patterson (1976) evaluated the integral $N_k(t)$ in (3.7.16) by expanding $T_k(x)$ as a series of Legendre functions and obtained the formula

$$\int_{-1}^1 f(x) e^{itx} dx \approx \sqrt{\frac{\pi}{2t}} \sum_{j=0}^n a_j \sum_{k=0}^j i^k (2k+1) R_{k,j} J_{k+1/2}(t), \quad (3.7.23)$$

where the recurrence relation to compute $R_{k,j}$ is given by

$$R_{k,j} = \int_{-1}^1 P_k(x) T_j(x) dx, \quad R_{k+2,j} = \left(\frac{j^2 + k^2}{j^2 - (k+3)^2} \right) R_{i,j}. \quad (3.7.24)$$

This method provides a stable approximation except that we need an efficient procedure to evaluate Bessel functions.

According to Alaylioglu, Evans and Hyslop (1976), to compute the integral $I_{\cos} = \int_a^b f(x) \cos(tx) dx$, we use a linear transformation of the form $x = \frac{(b+a) + (b-a)\xi}{2}$ which results in

$$I_{\cos} = \frac{b-a}{2} \int_{-1}^1 \left[\cos \frac{(b+a)w}{2} F(\xi) \cos(w\xi) - \sin \frac{(b+a)w}{2} F(\xi) \sin(w\xi) \right] d\xi, \quad (3.7.25)$$

where $w = (b-a)t/2$. If we approximate $F(\xi)$ by $F(\xi) \approx \sum_{i=0}^n a_i T_i(\xi)$, and collate at the $n+1$ nodes $\xi_j = \cos \frac{\pi j}{n}$, $j = 0, 1, \dots, n$, then we obtain

$$I_{\cos} \approx \frac{b-a}{2} \left[\cos \frac{(b+a)w}{2} \sum_{i=0}^n D_{i,m} \int_{-1}^1 \xi^m \cos(w\xi) d\xi - \sin \frac{(b+a)w}{2} \sum_{i=0}^n D_{i,m} \int_{-1}^1 \xi^m \sin(w\xi) d\xi \right], \quad (3.7.26)$$

where the coefficients $D_{i,m}$ are defined by the recurrence relation (1.2.11) for $T_n(x)$, and

$$a_i = \frac{2}{n} \sum_{j=0}^n F(\xi_j) \cos \frac{\pi j i}{n}.$$

Similarly,

$$\begin{aligned}
 I_{\sin} &= \int_a^b f(x) \sin(tx) dx \\
 &\approx \frac{b-a}{2} \left[\sin \frac{(b+a)w}{2} \sum_{i=0}^n {}''D_{i,m} \int_{-1}^1 \xi^m \cos(w\xi) d\xi \right. \\
 &\quad \left. - \cos \frac{(b+a)w}{2} \sum_{i=0}^n {}''D_{i,m} \int_{-1}^1 \xi^m \sin(w\xi) d\xi \right], \quad (3.7.27)
 \end{aligned}$$

where for the integrals we use the formula

$$\int_{-1}^1 \xi^m \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} (w\xi) d\xi = \pm \sum_{k=0}^m k! \binom{m}{n} \frac{\xi^{m-k}}{w^{k+1}} \begin{Bmatrix} \sin \\ \cos \end{Bmatrix} (w\xi + k\pi/2) \Big|_{-1}^1. \quad (3.7.28)$$

The series in (3.7.28) converges rapidly for large w provided $f(x)$ is smooth and has a fit by a Chebyshev series with small n . However, for small w and large n we may find instabilities. An alternative method to avoid this situation is to use the following series expansions:

$$\begin{aligned}
 \int_{-1}^1 x^m \cos(tx) dx &= 2 \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k+m+1)(2k)!} \quad m \text{ even}, \\
 \int_{-1}^1 x^m \sin(tx) dx &= 2 \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+m+2)(2k+1)!} \quad m \text{ odd}. \quad (3.7.29)
 \end{aligned}$$

The maximum value k_0 of k that gives precision accuracy up to 22 figures for these intervals is given roughly by $k_0 = 2w + 10$ (round-off to integer values), which for the truncation of the infinite series is reliable for $w \leq 10$. But for large values of w the situation is fluid; for example, $k_0 \approx 210$ for $w = 100$, although the actual maximum value of k turns out to be about 160. Thus, for such large values of w it is better to use formulas (3.7.28) instead of (3.7.29).

EXAMPLE 3.7.2. Compute

$$\int_0^{2\pi} x \cos x \sin(tx) dx = \begin{cases} -\frac{\pi}{2} & \text{for } t = 1, \\ -\frac{2\pi t}{t^2 - 1} & \text{for } t = 2, 3, \dots \end{cases}$$

The results are compared in [Table 3.7.2](#), which are obtained by Piessens and Poleunis formula (3.7.23) and by Alaylioglu, Evans and Hyslop formula (3.7.27). In the former case the number of function evaluations is 30, compared to 19 or 20 in the latter case

which also gives better results. ■

Table 3.7.2.

t	Exact	Formula (3.7.23) Absolute Error	Formula (3.7.27) Absolute Error
1	-1.5707963267948966	5(-15)	4(-16)
2	-4.1887902047863910	9(-15)	6(-16)
4	-1.6755160819145564	3(-15)	1(-15)
16	-0.3942390780975427	1(-14)	5(-15)
64	-0.0981987447275930	3(-15)	2(-16)
256	-0.0245440671189132	1(-15)	2(-16)

EXAMPLE 3.7.3. Compute $\int_{-1}^1 \cos(\pi p x^2) \cos(\pi q x) dx$, which has the exact value

$$\frac{1}{\sqrt{2p}} \left\{ \cos A[C(B_1) + C(B_2)] + \sin A[S(B_1) + S(B_2)] \right\},$$

where $A = \frac{\pi q^2}{4p}$, $B_{1,2} = \sqrt{\frac{2}{p}} \left(p \pm \frac{q}{2} \right)$, and $C(z)$ and $S(z)$ are the Fresnel integrals (Bakhvalov and Vasileva 1968). The results for the exact values and absolute errors for different values of n are presented in Table 3.7.3.

Table 3.7.3.

p	q	Exact	$n = 9$	$n = 15$	$n = 22$
$\frac{1}{4}$	$\frac{5}{4}$	-0.025816237030406	2.3(-8)	1.5(-13)	*
$\frac{1}{4}$	$\frac{41}{4}$	0.02966470953267	1.7(-7)	5.7(-12)	*
$\frac{1}{4}$	$\frac{451}{4}$	0.00283575769375	1.1(-9)	8.9(-14)	*
			$n = 34$	$n = 40$	$n = 47$
$\frac{23}{4}$	$\frac{5}{4}$	0.38215576878521	1.7(-8)	4.5(-12)	9.1(-13)
$\frac{23}{4}$	$\frac{41}{4}$	0.09736922562982	1.6(-5)	2.0(-8)	6.0(-12)
$\frac{23}{4}$	$\frac{451}{4}$	0.00256072719178	8.4(-8)	1.6(-10)	2.9(-12)
$\frac{47}{4}$	$\frac{5}{4}$	0.24111868127101	4.3(-5)	8.0(-6)	1.0(-7)
$\frac{47}{4}$	$\frac{41}{4}$	0.26746038313517	2.5(-2)	6.2(-4)	1.4(-8)
$\frac{47}{4}$	$\frac{451}{4}$	0.00233286903629	2.8(-4)	1.4(-4)	1.6(-5)

* exact in more than 22 digits.

3.7.3. Nontrigonometric Oscillatory Functions. Ehrenmark's formula (1968)

$$\int_0^{2h} f(x) dx = A_0 f(0) + 2A_1 f(h) + A_2 f(2h) + E, \quad (3.7.30)$$

which is of the Newton-Cotes type, is exact for $f(x) = 1$, $\sin(tx)$, and $\cos(tx)$, and for these functions $A_0 = A_2 = \frac{t h - \sin(th)}{t [1 - \cos(th)]}$, and $A_1 = h - A_0$. This formula can be used to compute integrals of the form $\int_a^b \cos(p \cos x - q \sin x) dx$, where p and q are constants. Its accuracy becomes more accurate with the increase in the number of subdivisions of the interval of integration, i.e., with the decrease in the step size h . There are three extensions to higher point numbers N , with the choice of $f(x)$ which, when used, makes the formula exact. These are the following sets $\{C_j(x)\}$:

- (i) $\sin(tx), \cos(tx), 1, x, x^2, \dots$,
- (ii) $1, \sin(tx), \cos(tx), \sin(2tx), \cos(2tx), \sin(3tx), \dots$, and
- (iii) $1, \sin(tx)/M, \cos(tx)/M, \sin(2tx)/M, \cos(2tx)/M, \sin(3tx)/M, \dots$,

where $M = [n/2]$. There are two choices for the nodes, one equally spaced to yield N-C type formulas and the other cosine-weighted nodes as in the Clenshaw-Curtis formulas. Most of these extensions are for the set (ii) where no particular choice is made for the nodes. Once these nodes are fixed, the weights w_i are determined by solving the system of linear algebraic equations

$$\int_a^b C_j(x) dx = c_j = \sum_{i=1}^n w_i C_j(x_i), \quad j = 1, \dots, n. \quad (3.7.31)$$

For integrands of the form $\sin k(\alpha t + \beta)$ a suitable transformation to change each subinterval to $[0, 2h]$ is required.

Levin's method (1982) to compute the oscillatory integrals of the form $I = \int_a^b f(x) e^{iq(x)} dx$ is based on assuming that $f(x)$ is of the form $f(x) = iq'(x)p(x) + p'(x)$, which is a linear ordinary differential equation and has the solution

$$p(x) = e^{-iq(x)} \left[\int_a^x f(t) e^{iq(t)} dt + c \right].$$

Then the integral I is evaluated directly to yield

$$I = p(b) e^{iq(b)} - p(a) e^{iq(a)}. \quad (3.7.32)$$

This means that the solution (3.7.32) is as oscillatory as the original integrand in I . But if both f and q are slowly oscillatory, then a slowly oscillatory solution $p_0(x)$ is obtained by substituting $p(x) = p_0(x) + c e^{-iq(x)}$ into (3.7.32); this solution is

$$I = p_0(b) e^{iq(b)} - p_0(a) e^{iq(a)}. \quad (3.7.33)$$

To compute $p_0(a)$ and $p_0(b)$, we take an n -point collocation to the basis set $\{u_k(x)\}$ for $k = 1, \dots, n$, so that when $p_0(x) = \sum_{k=1}^n \alpha_k u_k(x)$ is substituted into $f(x) = iq'(x)p(x) + p'(x)$, we obtain a system of n algebraic equations to evaluate α_k . Then I is computed from (3.7.33).

Evans (1992) has considered integrals of the form $\int_a^b f(x) J_n(tx) dx$, which are reduced to the form

$$\int_{-1}^1 y^j J_n(Ay + B) dy = \frac{1}{A^{j+1}} \int_{B-A}^{B+A} (z - B)^j J_n(z) dz, \quad (3.7.34)$$

where $A = (b - a)/2$, $B = (b + a)/2$, and $z = Ay + B$. These integrals are then evaluated by using the formula

$$\begin{aligned} \int_0^z t^\mu J_\nu(t) dt &= \frac{z^\mu \Gamma\left(\frac{\nu + \mu + 1}{2}\right)}{\Gamma\left(\frac{\nu - \mu + 1}{2}\right)} \\ &\times \sum_{k=0}^{\infty} \frac{(\nu + 2k + 1) \Gamma\left(\frac{\nu - \mu + 1}{2} + k\right)}{\Gamma\left(\frac{\nu + \mu + 3}{2} + k\right)} J_{\nu+2k+1}(z). \end{aligned} \quad (3.7.35)$$

While computing, one must be careful when combining the functions $\Gamma\left(\frac{\nu - \mu + 1}{2}\right)$ and $\Gamma\left(\frac{\nu - \mu + 1}{2} + k\right)$ since both become zero when their arguments are negative integers although their quotient is not singular. The expansion (3.7.35) becomes numerically unstable if $B \gg A$.

3.8. Noninterpolatory Product Integration

In connection with the product integration on the finite interval $[a, b]$, consider a class of n -point quadrature rule $Q_n(f)$ of degree at least $2n - 3$. It is known that such a quadrature rule is uniquely determined by one node x' and the corresponding weight w' . For a given node x' let us characterize all weights w for which the pair (x', w') generates a positive quadrature formula. Also, for each fixed node x' which is not a node of the Gaussian rule Q_{n-1}^G and for each negative weight w' , there exists a quadrature rule Q_n of degree $2n - 3$. If all nodes are contained in the interval $[a, b]$, then each such quadrature rule converges for all $f \in C^1[a, b]$. Thus, given a nonnegative weight function on $[-1, 1]$, a quadrature rule $Q_n \in \mathcal{P}_m$ is a linear

functional map of the type

$$Q_n(f) = \sum_{k=1}^n w_{kn} f(x_{kn}), \quad w_{kn} \in R, \quad -\infty < x_{1n} < x_{2n} \dots < x_{nn} < \infty, \quad (3.8.1)$$

$$\int_{-1}^1 w(x) f(x) dx = Q_n(f) + E_n(f), \quad (3.8.2)$$

$$E_n(x^l) \begin{cases} = 0 & \text{for } l = 1, \dots, m, \\ \neq 0 & \text{for } l = m + 1, \end{cases} \quad (3.8.3)$$

where x^l denotes a monomial, and E_n is the error functional of $Q_n(f)$. Let $\{Q_n\}$ define a sequence of quadrature formulas Q_n , $n = 1, 2, \dots$. Then Q_n is said to be a *positive quadrature rule* iff all weights $w_{kn} \geq 0$. Let Q_n^G denote a Gaussian rule using n nodes, with maximum degree $2n - 1$, and let $p_n(x)$ be orthogonal polynomials associated with Q_n^G and defined by

$$p_n(x) = a_n \prod_{k=1}^n (x - x_{kn}^G), \quad \int_{-1}^1 p_n(x) p_m(x) w(x) dx = \delta_{n,m},$$

where $a_n > 0$. According to Freud (1969) all quadrature rules Q_n of degree $\geq 2n - 2$ are positive, while a quadrature rule of degree $2n - 3$ may have at most one negative weight (Micchelli and Rivlin 1973). Förster (1992) has studied the convergence of the sequences $\{Q_n\}$ of degree $\geq 2n - 3$, and proved that for a function $f \in C[-1, 1]$ and for every node $x' \in R \setminus \{x_{1,n-1}^G, x_{2,n-1}^G, \dots, x_{n-1,n-1}^G\}$ and every $w > 0$, (i) there exists a unique rule Q_n of degree $\geq 2n - 3$ which has a node at x' and the associated weight w' ; (ii) all nodes of Q_n are contained in the interval $[\alpha, \beta]$, where $\alpha = \min\{y, x_{1,n-1}^G\}$ and $\beta = \max\{y, x_{n-1,n-1}^G\}$; (iii) $\liminf_{n \rightarrow \infty} |E_n(f)| > 0$ for a function $f \in C^1[-1, 1]$; (iv) if the each rule in the sequence $\{Q_n^G\}$ has degree $\geq 2n - 3$ and all nodes x_{kn} are contained in $[-1, 1]$, then $\lim_{n \rightarrow \infty} E_n(f) = 0$ for every function f which has absolutely continuous derivative f' on $[-1, 1]$; and (v) if $c_k(Q_n) = \sup_{\|f^{(k)}\| \leq 1} |E_n(f)|$ denotes the error constant of order k for $\|f^{(k)}\| = \sup_{|x| \leq 1} |f^{(k)}|$, then for all nonpositive rules Q_n of degree $\geq 2n - 3$, the error $E_n(f)$ is positive of degree $\geq 2n - 2$, and

$$c_{n-2}(Q_n) > c_{n-2}(Q_{n-1}^G), \quad \lim_{n \rightarrow \infty} \frac{c_{2n-2}(Q_n)}{c_{2n-2}(Q_{n-1}^G)} = 1.$$

Note that for the N-C rules Q_n^{NC} there exist analytic functions f on $[-1, 1]$ for which the sequence $\{Q_n^{NC}\}$ diverges (see Brass 1977).

Product integration provides an important aspect that is useful not only in quadrature rules but also in computation of integral equations (see §10.4). For a linear

interpolatory quadrature rule with positive weights, let S denote the set of nodes. According to Patterson (1969) there exists a set $T \subset S$ which contains $(n - 1)$ nodes such that the weights of the rule on T are all nonnegative. Thus, for any linear positive interpolatory (product) integration rule (PIIR) Q it is always possible to generate a sequence of imbedded PIIR's which start with Q . Let the integral $I_a^b(kf)$, where $-\infty \leq a < b \leq \infty$, be approximated by the PIIR's of the form $Q_n(f) = \sum_{i=1}^n w_{in} f(x_{in})$. These rules are exact for $f \in \mathcal{P}_{n-1}$. Then, given two distinct IIR's $Q_n(f)$ and $Q_m(f)$, with their respective nodes $X_n = \{x_{in} : i = 1, 2, \dots, n\}$, and $X_m = \{x_{im} : m = 0, 1, 2, \dots, m\}$, the rule $Q_m(f)$ is said to be *totally imbedded* in $Q_n(f)$ if $X_m \subset X_n$, and *partially imbedded* if $m < n$ and $X_m \cap X_n = \emptyset$. Rabinowitz et al. (1987) have proved that for any PIIR $Q_n(f)$ with the set of nodes X_n , there exists a finite set of PIIR's $\{Q_{n_k}(f); k = 1, 2, \dots, m \leq n\}$ such that (i) $Q_{n_1}(f) = Q_n(f)$, (ii) $Q_{n_{k+1}}(f)$ is imbedded in $Q_{n_k}(f)$, and this finite set of PIIR's is exact for $f \in \mathcal{P}_{n_k-2}$, $k = 1, 2, \dots, m - 1$. Also, if $[a, b]$ is a finite interval or $(-\infty, \infty)$, let $c = (b + a)/2$ or 0, respectively. Then the rule $Q_n(f)$ is said to be *symmetric* if $x_{in} + c = c - x_{n+1-i,n}$ and $w_{in} = w_{n+1-i,n}$ for $i = 1, 2, \dots, n$. Note that in such a symmetric case the PIIR rule $Q_n(f)$ is of precision n if n is odd. Also, there exists a finite sequence of imbedded symmetric PIIR's with the rule $Q_n(f)$ as the first element of this sequence, and each rule is of precision $\leq r - 3$, where r is the number of nodes in the previous rule in the sequence.

For a linear interpolatory quadrature rule with positive weights, let S denote the set of nodes. According to Patterson (1969) there exists a set $T \subset S$ which contains $(n - 1)$ nodes such that the weights of the rule on T are all nonnegative. Thus, for any linear positive interpolatory (product) integration rule (PIIR) Q it is always possible to generate a sequence of imbedded PIIR's which start with Q . Let the integral $I_a^b(kf)$, where $-\infty \leq a < b \leq \infty$, be approximated by the PIIR's of the form $Q_n(f) = \sum_{i=1}^n w_{in} f(x_{in})$. These rules are exact for $f \in \mathcal{P}_{n-1}$. Then, given two distinct IIR's $Q_n(f)$ and $Q_m(f)$, with their respective nodes $X_n = \{x_{in} : i = 1, 2, \dots, n\}$, and $X_m = \{x_{im} : m = 0, 1, 2, \dots, m\}$, the rule $Q_m(f)$ is said to be *totally imbedded* in $Q_n(f)$ if $X_m \subset X_n$, and *partially imbedded* if $m < n$ and $X_m \cap X_n = \emptyset$. Rabinowitz et al. (1987) have proved that for any PIIR $Q_n(f)$ with the set of nodes X_n , there exists a finite set of PIIR's $\{Q_{n_k}(f); k = 1, 2, \dots, m \leq n\}$ such that (i) $Q_{n_1}(f) = Q_n(f)$, (ii) $Q_{n_{k+1}}(f)$ is imbedded in $Q_{n_k}(f)$, and this finite set of PIIR's is exact for $f \in \mathcal{P}_{n_k-2}$, $k = 1, 2, \dots, m - 1$. Also, if $[a, b]$ is a finite interval or $(-\infty, \infty)$, let $c = (b + a)/2$ or 0, respectively. Then the rule $Q_n(f)$ is said to be *symmetric* if $x_{in} + c = c - x_{n+1-i,n}$ and $w_{in} = w_{n+1-i,n}$ for $i = 1, 2, \dots, n$. Note that in such a symmetric case the PIIR rule $Q_n(f)$ is of precision n if n is odd. Also, there exists a finite sequence of imbedded symmetric PIIR's with the rule $Q_n(f)$ as the first element of this sequence, and each rule is of precision $\leq r - 3$, where r is the number of nodes in the previous rule in the sequence.

The technique of product integration discussed here deals with the noninterpolatory (nonpolynomial) integration rules which are based on generalized piecewise

polynomial interpolation and modified moments. Product integration rules have been studied by Atkinson (1976), Dagnino (1983), de Hoog and Weiss (1973), Elliott and Paget (1976, 1978), Rabinowitz (1986, 1987), Lubinsky and Sidi (1986), Schneider (1981), Rabinowitz and Sloan (1984), Sloan (1980), Sloan and Smith (1978, 1980, 1982), Spence (1979), and Töpler and Volk (1980). Besides its use in integration of functions which are products of two functions, it has been applied in numerical solution of Fredholm integral equations of the second kind (see [Chapter 9](#)). We consider two functions $k \in L_1(a, b)$ and $f \in F[a, b]$ and define the approximation

$$I_a^b(kf) \approx I_n(f) = \sum_{i=1}^{m_n} w_{in} f(x_{in}), \quad (3.8.4)$$

such that $I_n(f) \rightarrow I_a^b(wf) = \int_a^b w(x) f(x) dx$ as $n \rightarrow \infty$ for all $f \in F[a, b]$, where $w \in A[a, b]$; here x_{in} are the zeros of $q_{n+\alpha+\beta}(x) = (1-x)^\alpha(1+x)^\beta p_n(x; w)$, $\alpha, \beta \in (0, 1)$, where $p_n(x; w)$ are orthonormal polynomials with respect to some $w \in A[a, b]$; and the moments $\int_a^b w(x) x^i dx < \infty$ for $i = 0, 1, \dots$ (for more on moments, see §4.4). We define the integration rules $\{Q_n(f)\}$ by

$$Q_n(f) = \sum_{i=1}^{m_n} w_{in}(x) f(x_{in}), \quad (3.8.5)$$

and determine the conditions on k , f , and the sequence $\{I_n(f)\}$, which guarantee that $Q_n(f) \rightarrow I_a^b(kf)$ as $n \rightarrow \infty$. The weights w_{in} are chosen such that (3.8.5) is exact for all $f \in \mathcal{P}_{n+\alpha+\beta-1}$. Sloan and Smith (1978, 1980, 1982) and Rabinowitz (1986) have shown that the sequence $\{Q_n(f)\}$ converges to $I_a^b(kf)$ for all $f \in F[a, b]$ or $f \in C[a, b]$, and that $|Q_n|(f) = \sum_{i=1}^{m_n} |w_{in}(k)| f(x_{in})$ converges to $I_a^b(|k|f)$.

Let

$$M_j(k) = \int_a^b w(x) K(x) p_j(x; w) dx, \quad (3.8.6)$$

denote the modified moments of k with respect to a given sequence of polynomials $p_j(x; w)$, where $K(x) = k(x)/w(x)$. We will define the *generalized piecewise polynomial product rule* (abbreviated GP³IR) as follows: Let the partition of the interval $[a, b]$ be $-\infty < a = t_0 < t_1 < \dots < t_n = b < \infty$; let $h_i = t_i - t_{i-1}$ for $i = 1, \dots, n$, and let $\Delta_n = \max h_i$. Similarly, we partition a subinterval $[t_{i-1}, t_i]$ by $t_{i-1} \equiv x_{i0} < x_{i1} < \dots < x_{i,m_i} \leq x_{i,m_i+1} \equiv t_i$, for $m_i \geq 1$. The points x_{ij} , $j = 1, \dots, m_i$, are called the grid points (abscissae or nodes). Two grid points are coincident if $x_{i,m_i} = t_i = x_{i+1,m_i}$. Define $h_{ij} = x_{i,j+1} - x_{ij}$, $j = 0, 1, \dots, m_i$. Note that $h_{i0} = 0$ if $x_{i1} = t_{i-1}$, and $h_{i,m_i} = 0$ if $x_{i,m_i} = t_i$. Then the *product integration rule* is

$$Q_n(f) = \sum_{i=1}^n \sum_{j=1}^{m_i} w_{ij} f_{ij}, \quad f_{ij} = f(x_{ij}), \quad (3.8.7)$$

$$w_{ij} = \int_{t_{i-1}}^{t_i} l_{ij} k(x) dx, \quad i = 1, \dots, n; \quad j = 1, \dots, m_i, \quad (3.8.8)$$

$$l_{ij} = \prod_{\substack{k=1 \\ k \neq j}}^{m_i} \frac{x - x_{ik}}{x_{ij} - x_{ik}}, \quad (3.8.9)$$

where l_{ij} are the fundamental Lagrange polynomials. Alternatively, Rabinowitz (1987) defines this product integration rule by

$$Q_n(f) = \sum_{i=1}^n \int_{t_{i-1}}^{t_i} k(x) L_i(x) dx, \quad (3.8.10)$$

where $L_i(x) = \sum_{j=1}^{m_i} l_{ij}(x) F_{ij}$. It is shown that if

$$p_n(x) = \begin{cases} L_i(x) & \text{if } t_{i-1} < x \leq t_i, \\ L_1(a) & \text{if } x = a, \end{cases}$$

then $Q_n(f) = I_a^b(k p_n)$, where p_n is a piecewise polynomial in the class \mathcal{P}_{M_n-1} , and $M_n = \max_{1 \leq i \leq n} m_i$. Moreover, if $x_{i,m_i} = t_i = x_{i+1,1}$ for $1 \leq i \leq n-1$, then $p_n \in C[a, b]$. However, it is noted that in the case of a general distribution of the nodes x_{ij} , a rule $Q_n(f)$ may fail to converge to $I_a^b(kf)$, even if $f \in C[a, b]$ and $k \equiv 1$, $\Delta_n \rightarrow 0$ and M_n is bounded. The reason for such a case is that the polynomials $l_{ij}(x)$ may not be uniformly bounded for large n in an interval $[t_{i-1}, t_i]$. But if

$$|l_{ij}(x)| \leq L, \quad x \in [t_{i-1}, t_i] \quad \text{for all } i, j, n, \quad (3.8.11)$$

then we have (i) $h_{ij} \geq c h_i$ for a constant $c \in (0, 1)$ for all $i = 1, \dots, n$ and $j = 1, \dots, m_i$, and (ii) $M_n \leq \overline{M}$ for all n . Then

$$|l_{ij}(x)| = \left| \prod_{\substack{k=1 \\ k \neq j}}^{m_i} \frac{x - x_{ik}}{x_{ij} - x_{ik}} \right| \leq \frac{h_i^{m_i-1}}{(c h_i)^{m_i-1}} \leq \frac{1}{c^{\overline{M}-1}} \equiv L, \quad t_{i-1} \leq x \leq t_i. \quad (3.8.12)$$

Then, in view of the condition (3.8.11), we have

$$|w_{ij}| = \left| \int_{t_{i-1}}^{t_i} l_{ij}(x) k(x) dx \right| \leq L \int_{t_{i-1}}^{t_i} |k(x)| dx. \quad (3.8.13)$$

A sequence of rules (3.8.7) is called a sequence of GP³IR if (i) $h_{ij} \geq c h_i$ for $c \in (0, 1)$, $i = 1, \dots, n$ and $j = 1, \dots, m_i$, (ii) $\Delta_n \rightarrow 0$ as $n \rightarrow \infty$, and (iii) $M_n \leq \overline{M}$ for all n . For such a sequence, $Q_n(f) \rightarrow I_a^b(kf)$ for all $f \in C[a, b]$

and for all $f \in P[a, b]$ (Rabinowitz and Sloan 1984), and $Q_n(f) \rightarrow I_a^b(kf)$ for all $f \in R[a, b]$ (Rabinowitz 1987).

3.8.1. Approximation by Fourier Series. A sequence of integration rules $\{I_n(f)\}$ associated with the weight function $w(x) \in A[a, b]$ such that $I_n(f) \rightarrow I_a^b(wf)$ for all $f \in F[a, b]$ is obtained by approximating f by a finite part of its Fourier series expansion in the orthonormal polynomials $p_n(x; w)$:

$$f(x) \approx \sum_{j=0}^N a_j p_j(x; w), \quad (3.8.14)$$

where $a_j = \langle f, p_j \rangle$. If we replace a_j by

$$\hat{a}_{jn} = I_n(f p_j) = \sum_{i=1}^{m_n} w_{in} f(x_{in}) p_j(x_{in}; w), \quad (3.8.15)$$

then

$$I_a^b(kf) \approx \sum_{j=0}^N \hat{a}_{jn} M_j(k) \equiv Q_n^N(f), \quad (3.8.16)$$

where $M_j(k)$ are given by (3.8.6). If we use orthogonal polynomials instead of orthonormal polynomials, we must divide a_j by $\langle p_j, p_j \rangle$ and \hat{a}_{jn} by h_j . The recurrence relations for $M_j(k)$ for different types of functions $K(x) = k(x)/w(x)$ on $[-1, 1]$, with $w(x) = (1 - x^2)^{-1/2}$ and $p_j(x; w) = T_n(x)$ are given in Piessens and Branders (1973, 1975, 1976, 1983). Modified moments $M_j(k)$ (see §4.4.10) are exactly the Fourier coefficients of $K(x)$. In particular, the modified moments with $w(x) = 1$ and $p_j(x) = P_j(x)$ (Legendre polynomials) on $[-1, 1]$ coincide with the Fourier coefficients; for $w(x) = (1 - x)^\alpha(1 + x)^\beta$ (Jacobi weight function), Paget (1976) gives formulas for the Fourier coefficients of (i) $K(x; \lambda) = e^{i\lambda x}$, where λ is real; (ii) $K(x; \lambda) = \log|x - \lambda|$, $-1 < \lambda < 1$; and (iii) $K(x, \lambda) = |x - \lambda|^s$, $s > -1$, $-1 < \lambda < 1$; and also an algorithm to compute the sum $\sum c_j M_j(wk)$. Additional modified moments with Jacobi and Legendre polynomials are available in Gatteschi (1980). In all cases, $Q_n^N(f)$ is exact for all $f \in \mathcal{P}_{n-1}$.

Let $L_{2,w}$ denote the weighted L_2 normed space defined by $L_{2,w} = \{g : \|g\|_{2,w} < \infty\}$, and F denote a family of functions defined on the finite or infinite interval $[a, b]$ such that $f \in F[a, b]$ is either $f \in C[a, b]$ or $f \in R[a, b]$. Suppose that $w \in A[a, b]$, $K \in L_{2,w}[a, b]$, and $f \in L_{2,w}[a, b] \cap F[a, b]$. If $I_n(f p_j) \rightarrow \langle f, p_j \rangle$ for all j and for all $f \in F[a, b]$, then

$$\lim_{N \rightarrow \infty} \lim_{n \rightarrow \infty} Q_n^N(f) = I_a^b(kf). \quad (3.8.17)$$

This result is proved in Rabinowitz (1987), where two other results on double limits are also given. The first one concerns the generalized smooth Jacobi weight function

on $[-1, 1]$, which is defined by $w(x) = \psi(x)(1-x)^\alpha(1+x)^\beta \prod_{k=1}^m |t_k - x|^{\gamma_k}$, where $-1 < t_1 < \dots < t_m < 1$; $\alpha, \beta, \gamma_k > -1$ for $k = 1, \dots, m$; and $\psi > 0$ such that $\int_0^1 w(\psi; t) t^{-1} dt < \infty$. For this $w(x)$, let $v(x) = (1-x)^A(1+x)^B \prod_{k=1}^m |t_k - x|^{C_k}$, where $A = -\max\{(2\alpha+1)/4, 0\}$, $B = -\max\{(2\beta+1)/4, 0\}$, $C = -\max\{\gamma_k/2, 0\}$ for $k = 1, \dots, m$. Let $kv \in L_p[a, b]$ for some $p \in (1, \infty)$, and let $f/v \in L_q[a, b]$, where $p^{-1} + q^{-1} = 1$. Then (3.8.17) holds if $f \in F[a, b]$, and $I_n(fp_j) \rightarrow \langle f, p_j \rangle$ for all j and all $f \in F[a, b]$. The other result concerns the partial sum $S_N K(x) = \sum_{j=0}^N a_j K(x)$ which converges to $K(x)$ in $[a, b]$. The (3.8.17) holds if $I_n(gp) \rightarrow I_a^b(wgp)$ for all $g \in F[a, b]$ and all polynomials p , if $\sum_{i=1}^{m_n} |w_{in}| \leq B$ for all n , and if $f \in F[a, b]$ is bounded and $\sup |f| = M_f$.

3.8.2. Asymptotic Error Estimates. We will derive some error estimates for the Gaussian rule

$$I_{-1}^-(wf) = \sum_{k=1}^n w_k f(x_k) + E_n(f), \quad (3.8.18)$$

where the nodes x_k are the zeros of a polynomial $p_n(x)$ of degree n with the leading coefficient k_n , the weights w_k are given by $w_k = \int_{-1}^1 w(x) \frac{p_n(x)}{(x-x_n) p_n'(x)} dx$, and the error by $E_n(f) = \frac{f^{2n}(\xi)}{(2n)! k_n^2}$, (see [Davis and Rabinowitz 1984](#), p. 305). If we define $q_n(z) = \int_{-1}^1 w(x) \frac{p_n(x)}{z-x} dx$, $z \notin [-1, 1]$, then

$$E_n(f) = \frac{1}{2i\pi} \int_{\Gamma} \frac{q_n(z)}{p_n(z)} f(z) dz,$$

where Γ is a closed contour in \mathcal{C} containing $[-1, 1]$, $f(z)$ is analytic in \mathcal{C} , and w and $|\log w|$ belong to the class $R[-1, 1]$. By using the mapping $z = \frac{1}{2}(\xi + \xi^{-1})$, which maps the circle $|z| = \rho > 1$ in the ξ -plane onto the ellipse \mathcal{E}_ρ in the z -plane with foci at ± 1 and the semi-axes $\frac{1}{2}(\rho + \rho^{-1})$, and for the inverse mapping choosing the sign of the square root such that $|\xi| > 1$ for $z \notin [-1, 1]$, we find that on any compact support of $\mathcal{C} \setminus [-1, 1]$

$$\frac{q_n(z)}{p_n(z)} = 2\pi \xi^{-2n-1} D(\xi^{-1}; w) (1 + o(1)) \quad \text{as } n \rightarrow \infty, \quad (3.8.19)$$

where $|\xi| > 1$, and

$$D(\xi^{-1}; w) = \exp \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} \log [w(\cos \theta)] \frac{1 + \xi^{-1} e^{-i\theta}}{1 - \xi^{-1} e^{-i\theta}} d\theta \right\} \quad (3.8.20)$$

$$= \xi^{-k} \exp \left\{ \frac{1}{\pi} \int_0^{\pi} \log [w(\cos \theta)] d\theta \right\} \exp \left\{ \frac{2}{\pi} \sum_{k=1}^{\infty} \log [w(\cos \theta)] \cos k\theta d\theta \right\}. \quad (3.8.21)$$

Some properties of $D(\xi^{-1}; w)$ are:

- (i) $D(\xi^{-1}; w_1 w_2) = D(\xi^{-1}; w_1) D(\xi^{-1}; w_2)$;
- (ii) $D(\xi^{-1}; w_1/w_2) = D(\xi^{-1}; w_1) / D(\xi^{-1}; w_2)$,
- (iii) $D(\xi^{-1}; w^p) = D(\xi^{-1}; w)^p$ for constant p ,
- (iv) $D(\xi^{-1}; k) = k$ for scalar k , and
- (v) $D(\xi^{-1}; k w_1) = k D(\xi^{-1}; w_1)$ for scalar k . Also,

$$\int_0^{\pi} \log [w(\cos \theta)] \cos k\theta d\theta = -\frac{\pi}{k} \sum_j \xi_{\alpha_j}^{-k} r_j, \quad (3.8.22)$$

for $k = 1, 2, \dots$, $\xi_{\alpha_j} = \alpha_j + \sqrt{\alpha_j^2 - 1}$, $|\xi_j| > 1$, and $r_j = \text{Res}_{z=\alpha_j} \left[\frac{w'(z)}{w(z)} \right]$.

Thus, Chen (1982) proves that

$$D(\xi^{-1}; w) = e^{A_0} \prod_j \left(1 - \xi_{\alpha_j}^{-1} \xi^{-1} \right)^{r_j} \quad \text{for } |\xi| > 1, \quad (3.8.23)$$

where $A_0 = \frac{1}{\pi} \int_{-1}^1 \frac{\log [w(z)]}{\sqrt{1-x^2}} dx$. Some special cases are:

1. If $w(x) = (1+x)^m (1-x)^n w_1(x)$ for some nonnegative constants m, n , and $w_1(\pm 1) \neq 0$, then

$$D(\xi^{-1}; w) = 2^{-m-n} (1 + \xi^{-1})^{2m} (1 - \xi^{-1})^{2n} D(\xi^{-1}; w_1).$$

Thus, $D(\xi^{-1}; w)$ for the Gauss-Jacobi rule is obtained by setting $m = \alpha$ and $\beta = n$.

2. If $w(x) = 1/(x^2 + a^2)$ for $a > 0$, then

$$D(\xi^{-1}; w) = \frac{4}{(a + \sqrt{a^2 + 1}) \left[1 + \frac{(\sqrt{a^2 + 1} - a)^2}{\xi^2} \right]^2}. \quad (3.8.24)$$

3. If $w(x) = 1/(x + a)$ for real $|a| > 1$, then

$$D(\xi^{-1}; w) = \frac{2}{(a + \sqrt{a^2 + 1}) \left[1 + \frac{a - \sqrt{a^2 + 1}}{\xi} \right]^2}. \quad (3.8.25)$$

Finally, in view of (3.8.19) we find that

$$E_n(f) \approx i \int_{\Gamma} e^{h(z)} D\left(\xi^{-1}; w\right) dz. \tag{3.8.26}$$

We consider the following cases.

CASE 1. if f is an entire function, then from (3.8.26) we get

$$\begin{aligned} E_n(f) &\approx -i \sqrt{2\pi} \frac{\alpha}{\sqrt{|h''(z_0)|}} e^{h(z_0)} D\left(\xi^{-1}; w\right) \\ &\approx \frac{i\alpha}{\sqrt{2\pi} \sqrt{|h''(z_0)|}} e^{h(z_0)+A_0} \prod_j \left(1 - \xi_{\alpha_j}^{-1} \xi_0^{-1}\right)^{r_j}, \end{aligned} \tag{3.8.27}$$

where $h(z) = \log[f(z)] - (2n + 1) \log[z + \sqrt{z^2 - 1}]$; $z_0 \notin [-1, 1]$ is a simple zero of $h'(z)$; $\xi_0 = z_0 + (z_0^2 - 1)$; $|\alpha| = 1$ and $\arg\{\alpha\} = \frac{1}{2} [\pi - \arg\{h''(z_0)\}]$; and α_j are simple poles of w'/w . There are two saddle points at $\pm \sqrt{(2n + 1)^2 + 1}$, of which the negative saddle point can be neglected because its contribution is relatively small.

EXAMPLE 3.8.1. Let $w(x) = e^x$, $f(x) = 1/(x^2 + a^2)$, and $a = 0.01$. Using the Gaussian rule (3.8.18), we find from (3.8.24) and (3.8.27) that

$$E_n(f) \approx \frac{4}{(a + \sqrt{a^2 + 1})^2} \sqrt{\frac{2\pi}{z_0}} e^{z_0} \xi_0^{-2n-1} \left[1 + \left(\sqrt{1 + a^2} - a\right)^2 \xi_0^{-2}\right]^{-2}.$$

The values of $|E_n(f)|$, both exact and computed from the above formula, are presented in Table 3.8.1. ■

Table 3.8.1. Values of $|E_n(f)|$. Table 3.8.2.

n	Exact	Approx.		Exact	Approx.
3	0.2474(−3)	0.2762(−3)		0.6887(−1)	0.7446(−1)
4	0.1132(−5)	0.1227(−5)		0.1219(−1)	0.1278(−1)
5	0.3186(−8)	0.3396(−8)		0.2109(−2)	0.2193(−2)
6	0.6091(−11)	0.6413(−11)		0.3644(−3)	0.3762(−3)

CASE 2. If $f(z)$ has simple poles at α_j , $j = 1, 2, \dots$, then by (3.8.22)

$$E_n(f) \approx -2\pi \sum_j D\left(\xi^{-1}; w\right) \xi_j^{-2n} r_j. \tag{3.8.28}$$

EXAMPLE 3.8.2. Let $f(x) = 1/(x^2 + 1)$, $w(z) = 1/(x^2 + a^2)$, and $a = 0.1$. The integrand (wf) has two simple poles at $\pm i$. Then from (3.8.24) and (3.8.28) we

get

$$E_n(f) \approx (-1)^{n+1} \frac{8\pi (1 + \sqrt{2})^{-2n-1}}{(a + \sqrt{a^2 + 1})^2} \left(\frac{1 - (\sqrt{1 + a^2} - a)^2}{3 + 2\sqrt{2}} \right)^{-2}.$$

The results for $|E_n(f)|$ are presented in Table 3.8.2. ■

CASE 3. If $f(z)$ has an algebraic singularity on the real axis, e.g., $f(z) = (c - z)^\mu g(z)$, $c > 1$, g an entire function, and μ a rational nonintegral constant, then

$$\begin{aligned} E_N(f) &\approx -2 \sin(\mu\pi) \lim_{a \rightarrow \infty} \int_c^a \frac{|c - x|^\mu g(x) D(\xi^{-1}; w)}{(x + \sqrt{x^2 - 1})^{2n+1}} dx \\ &= -2 \sin(\mu\pi) (c^2 - 1)^{(\mu+1)/2} \frac{g(c) \Gamma(\mu + 1) D(\xi^{-1}; w)}{(2n + 1)^{\mu+1} \xi_c^{2n+1}}, \end{aligned} \quad (3.8.29)$$

where $\xi_c = c + \sqrt{c^2 + 1}$, $|\xi_c| > 1$.

EXAMPLE 3.8.3. Let $w(x) = 1/(x + a)$, $f(x) = \sqrt{2 - x}$, and $a = 1.01$. The exact solution is

$$\int_{-1}^1 \frac{\sqrt{2 - x}}{x + a} dx = 2(1 - \sqrt{3}) - b \log \left[\frac{(\sqrt{3} - b)(1 + b)}{(\sqrt{3} + b)(1 - b)} \right],$$

where $b = \sqrt{2 + a}$. Then from (3.8.25) and (3.8.29) we get

$$E_n(f) \approx -\frac{2(27)^{1/4} \sqrt{\pi} (2n + 1)^{-3/2}}{a + \sqrt{a^2 - 1}} \left(1 + \frac{a - \sqrt{a^2 - 1}}{\xi_c} \right)^{-2} \xi_c^{-2n-1},$$

where $\xi_c = 2 + \sqrt{3}$. The result for $|E_n(f)|$ are presented in Table 3.8.3. ■

Table 3.8.3. Values of $|E_n(f)|$. Table 3.8.4.

n	Exact	Approx.		Exact	Approx.
3	0.3517(−4)	0.2472(−4)		0.2069(−3)	0.1762(−3)
4	0.1590(−5)	0.1218(−5)		0.1111(−4)	0.9839(−5)
5	0.8020(−7)	0.6470(−7)		0.6373(−6)	0.5780(−6)
6	0.4327(−8)	0.3616(−8)		0.3794(−7)	0.3511(−7)

CASE 4. If $f(z)$ has a logarithmic singularity on the real axis, e.g., $f(z) = g(z) \log(c - z)$, $c > 1$, and $g(z)$ entire, then

$$\begin{aligned} E_n(f) &\approx -2\pi \lim_{a \rightarrow \infty} \int_c^a g(x) D(\xi^{-1}; w) (x + \sqrt{x^2 - 1})^{-2n-1} dx \\ &\approx -\frac{2\pi g(c) \sqrt{c^2 - 1} D(\xi^{-1}; w)}{(2n + 1) \xi_c^{2n+1}}, \end{aligned} \quad (3.8.30)$$

where $\xi_c = c + \sqrt{c^2 - 1}$, and $|\xi_c| > 1$.

EXAMPLE 3.8.4. Let $w(x) = 1/(x + a)$, $f(x) = \log(2 - x)$, and $a = 1.01$. Then from (3.8.25) and (3.8.30) we get

$$E_n(f) \approx -\frac{4\pi\sqrt{3}\xi_c^{-2n-1}}{(2n+1)\left(a + \sqrt{a^2 - 1}\right)\left[1 + \frac{a - \sqrt{a^2 - 1}}{\xi_c}\right]^2},$$

where $\xi_c = 2 + \sqrt{3}$. The results for $|E_n(f)|$ are presented in Table 3.8.4. ■

EXAMPLE 3.8.5. Let $w(x) = e^{-x^2}$, $f(x) = e^{x^2}$, so that $w'/w = -2x$ is entire. Then $D(\xi^{-1}; w) = e^{-(1+\xi^{-2})/2}$. So as in Case 1, we have

$$E_n(f) \approx \sqrt{\frac{2\pi}{h''(z_0)}\xi_0^{2n+1}}\xi_0^{-2n-1}e^{z_0^2-(1+\xi_0^2)/2},$$

where $z_0 = \frac{\sqrt{2+2\sqrt{4n^2+4n+2}}}{2}$, $\xi_0 = z_0 + \sqrt{z_0^2 - 1}$, and $h''(z_0) = 2 + 8(2n+1)z_0[-2+2\sqrt{4n^2+4n+2}]^{3/2}$. There are two saddle points at $\pm z_0$, and the error estimate from both of them is

$$E_n(f) \approx \sum \sqrt{\frac{2\pi}{h''(z_0)}}\xi_0^{-2n-1}e^{z_0^2-(1+\xi_0^2)/2},$$

where the ‘sum’ is taken for both saddle points. The results of the values of $|E_n(f)|$ are presented in Table 3.8.5. ■

Table 3.8.5. Values of $|E_n(f)|$.

n	Exact	Approx.
3	0.6839(−2)	0.6105(−2)
4	0.4471(−3)	0.4734(−3)
5	0.2295(−4)	0.2779(−4)

3.9. Test Integrals

TABLE 1: TEST INTEGRALS OF KAHANER (1971):

$$1. \int_0^1 e^x dx = e - 1 \approx 1.718281828$$

2. $\int_0^1 \begin{cases} 0, & 0 \leq x < 0.3 \\ 1, & 0.3 \leq x \leq 1 \end{cases} dx = 0.7$
3. $\int_0^1 x^{1/2} dx = 2/3$
4. $\int_{-1}^1 \left(\frac{23}{25} \cosh x - \cos x \right) dx = \frac{46}{25} \sinh(1) - 2 \sin(1) \approx 0.479428266$
5. $\int_{-1}^1 (x^4 + x^2 + 0.9)^{-1} dx \approx 1.582232997$
6. $\int_0^1 x^{3/2} dx = 0.4$
7. $\int_0^1 x^{-1/2} dx = 2$
8. $\int_0^1 (1 + x^4)^{-1} dx \approx 0.866972987$
9. $\int_0^1 2/(2 + \sin(10\pi x)) dx = 2/\sqrt{3} \approx 1.154700538$
10. $\int_0^1 (1 + x)^{-1} dx = \ln 2 \approx 0.6931471806$
11. $\int_0^1 (1 + e^x)^{-1} dx = 1 + \ln 2 - \ln(1 + e) \approx 0.379885493$
12. $\int_0^1 x/(e^x - 1) dx \approx 0.777504634$
13. $\int_{0.1}^1 \sin(100)/\pi x dx = \ln(10) \sin(100)/\pi \approx 0.009098645257$
14. $\int_0^{10} \sqrt{50} e^{-50\pi x^2} dx = 0.5 \operatorname{erf}\left(50\sqrt{2\pi}\right) = 0.5$
15. $\int_0^{10} 25 e^{-25x} dx = 1 - e^{-250} \approx 1$
16. $\int_0^{10} 50/(\pi(1 + 2500x^2)) dx = \tan^{-1}(500)/\pi \approx 0.49936338107$
17. $\int_{0.01}^1 (\sin(50\pi x))^2 / (50\pi x)^2 dx$
 $= [\pi \operatorname{Si}(100\pi) - (\pi \operatorname{Si}(\pi) - 2)] / (50\pi^2) \approx 0.11213930827$
18. $\int_0^\pi \cos(\cos x + 3 \sin x + 2 \cos(2x) + 3 \cos(3x) + 3 \sin(2x)) dx$
 ≈ 0.8386763426
19. $\int_0^1 \ln x dx = -1$

20. $\int_{-1}^1 (x^2 + 1.005)^{-1} \, dx \approx 1.56439645$
21. $\int_0^1 (\operatorname{sech}^2(10(x - 0.2)) + \operatorname{sech}^4(100(x - 0.4))$
 $+ \operatorname{sech}^8(1000(x - 0.6))) \, dx \approx 0.2108027355$

TABLE 2: TEST INTEGRALS OF CASSALETTO, PICKET AND RICE (1969):
We use the notation: $F_k(x) = \sum_{j=0}^{n-1} (-1)^j (j+1) x^{k-j-1}$.

1. $\int_0^1 F_1(x) \, dx = 1$
2. $\int_0^1 F_2(x) \, dx = -3/2 = -1.5$
3. $\int_0^1 F_3(x) \, dx = 7/3 \approx 2.33333333333333$
4. $\int_0^1 F_4(x) \, dx = -35/12 \approx -2.91666666666666$
5. $\int_0^1 F_5(x) \, dx = 37/10 = 3.7$
6. $\int_0^1 F_6(x) \, dx = -259/60 \approx -4.31666666666666$
7. $\int_0^1 F_7(x) \, dx = 533/105 \approx 5.076190476190476$
8. $\int_0^1 F_8(x) \, dx = -1599/280 \approx -5.710714285714285$
9. $\int_0^1 F_9(x) \, dx = 1627/252 \approx 6.456349206349207$
10. $\int_0^1 F_{10}(x) \, dx = -17897/2520 \approx -7.101984126984127$
11. $\int_0^1 F_{11}(x) \, dx = 18107/2310 \approx 7.838528138528138$
12. $\int_0^1 F_{12}(x) \, dx = -235391/27720 \approx -8.49173881673882$
13. $\int_0^1 F_{13}(x) \, dx = 237371/25740 \approx 9.22187257187257$
14. $\int_0^1 F_{14}(x) \, dx = -237371/24024 \approx -9.88057775557776$

15. $\int_0^1 F_{15}(x) dx = 95549/9009 \approx 10.6059496059496$
16. $\int_0^1 F_{16}(x) dx = -1624333/144144 \approx -11.26882145632146$
17. $\int_0^1 F_{17}(x) dx = 1632341/136136 \approx 11.99051683610507$
18. $\int_0^1 F_{18}(x) dx = -31014479/2450448 \approx -12.65665666033313$
19. $\int_0^1 F_{19}(x) dx = 155685007/11639628 \approx 13.37542806350856$
20. $\int_0^1 F_{20}(x) dx = -155685007/11085360 \approx -14.04419946668399$
21. $\int_0^1 e^{-x} dx = 1 - 1/e \approx 0.6321205588285578$
22. $\int_0^1 \sin \pi x dx = 2/\pi \approx 0.6366197723675814$
23. $\int_0^1 \cos x dx = \sin(1) \approx 0.841470984807897$
24. $\int_0^1 x/(e^x - 1) dx = \pi^2/6 - 1 + \ln(e - 1) - Li_2(1/e)$
 $\approx 0.7775046341122486$
25. $\int_0^1 (1 + x^2)^{-1} dx = \pi/4 \approx 0.7853981633974463$
26. $\int_0^1 2/(2 + \sin(10\pi x)) dx = 2/\sqrt{3} \approx 1.154700538383864$
27. $\int_0^1 (1 + x^4)^{-1} dx = \frac{1}{2\sqrt{2}} \left[\frac{1}{2} \ln \frac{2 + \sqrt{2}}{2 - \sqrt{2}} + \frac{\pi}{2} \right] \approx 0.866972987339911$
28. $\int_0^1 (1 + e^x)^{-1} dx = 1 + \ln 2 - \ln(1 + e) \approx 0.3798854930417225$
29. $\int_0^{2\pi} x \sin(30x) \cos x dx = -60\pi/899 \approx -0.209672479661623$
30. $\int_0^{2\pi} x \sin(30x) \cos(50x) dx = 3\pi/80 \approx 0.1178097245099276$
31. $\int_0^{2\pi} x \sin(30x)/\sqrt{1 - x^2/(4\pi^2)} dx = 2\pi^3 J_1(60\pi)$
 $\approx -2.543259618893547$
32. $\int_{-1}^1 ((23/25) \cosh x - \cos x) dx = 46 \sinh(1)/25 - 2 \sin(1)$
 $\approx 0.4794282266888018$

$$33. \int_{-1}^1 (x^4 + x^2 + 0.9)^{-1} dx \approx 1.582232963729353$$

$$34. \int_{-1}^{100\pi} ((100\pi)^2 - x^2)^{-1/2 \sin x} dx = 50\pi^2 H_1(100\pi) \\ \approx 298.4357164943787$$

$$35. \int_0^1 (1+x)^{-1} dx = \ln 2 \approx 0.693147180559947$$

$$36. \int_0^1 x^{1/2} dx = 2/3 \approx 0.6666666666667$$

$$37. \int_0^1 x^{1/4} dx = 0.8$$

$$38. \int_0^1 x^{1/8} dx = 8/9 \approx 0.88888889$$

$$39. \int_0^1 x^{1/6} dx = 6/7 \approx 0.857142857143454$$

$$40. \int_0^1 (|x^2 - 0.25|)^{1/2} dx = \frac{\pi}{16} + \frac{1}{8} (2\sqrt{3} - \ln 2 - \ln(2 + \sqrt{3})/2) \\ \approx 0.4647425535922633$$

$$41. \int_0^1 x^{3/2} dx = 0.4$$

$$42. \int_0^1 (|x^2 - 0.25|)^{3/2} dx = \frac{3\pi}{256} + \frac{3}{128} (2\sqrt{3} + \ln 2 + \ln(2 + \sqrt{3})/2) \\ \approx 0.1488716206553019$$

$$43. \int_0^1 x^{5/2} dx = 2/7 \approx 0.2857142856503935$$

$$44. \int_0^1 (|x^2 - 0.25|)^{5/2} dx = \frac{5\pi}{2048} + \frac{1}{1024} (38\sqrt{3} - 5\ln 2 - 5\ln(2 + \sqrt{3})/2) \\ \approx 0.06551476838416691$$

$$45. \int_0^1 [10x] dx = 4.5$$

$$46. \int_0^1 \begin{cases} x, & 0 \leq x \leq 1/3 \\ x+1, & 1/3 \leq x \leq 2/3 \\ x+2, & 2/3 \leq x \leq 1 \end{cases} dx = 1.5$$

$$47. \int_0^1 \begin{cases} 0, & 0.49 < x < 0.5 \\ -1000(x^2 - x), & \text{otherwise} \end{cases} dx \approx 164.17195$$

$$48. \int_0^1 \begin{cases} 1/(x+2), & 0 \leq x \leq e-2 \\ 0, & e-2 \leq x \leq 1 \end{cases} dx \\ = 1 - \ln 2 \approx 0.3068528194400546$$

49. $\int_0^1 (10x-)(10x-1.1)(10x-1.2)(10x-1.3) \, dx$
 $= 1627879/1500 \approx 1085.252666666667$

50. $\int_0^1 \sin(100\pi x) \, dx = 0$

Comparison of Results.

- Legend:
 S_A : Compound Simpson's Rule with the number of correct digits;
 S_N : Compound Simpson's Rule with the number of digits needed for 10 figures accuracy;
 L_A : Compound Gauss-Legendre Rule with the number of correct digits;
 L_N : Compound Gauss-Legendre Rule with the number of digits needed for 10 figures accuracy;
 P_A : Patterson's Rule with the number of correct digits;
 P_N : Patterson's Rule with the number of digits needed for 10 figures accuracy;
 C_A : Clenshaw-Curtis Rule with the number of correct digits;
 C_N : Clenshaw-Curtis Rule with the number of digits needed for 10 figures accuracy.
 \times : Failed to reach 10-digit accuracy.
 $-$: Failed to run at all.

Table 3.9.1. Kahaner (1971) Test Integrals Set.

Integral	S_A	S_N	L_A	L_N	P_A	P_N	C_A	C_N
1	8	65	14	4	14	7	14	9
2	1	\times	1	\times	1	\times	1	\times
3	3	\times	4	\times	4	255	4	\times
4	7	\times	14	8	4	7	14	9
5	7	65	12	32	10	15	9	33
6	5	\times	7	64	8	63	7	65
7	-	-	1	\times	1	\times	-	-
8	6	\times	14	16	14	15	12	17
9	10	17	1	\times	2	255	2	257
10	7	65	14	8	15	12	14	17
11	9	33	14	8	14	7	14	9
12	9	33	14	8	14	7	14	9
13	0	\times	0	\times	0	\times	0	\times
14	0	\times	0	128	0	127	0	129
15	0	\times	0	64	2	63	0	65
16	0	\times	0	\times	1	255	1	257
17	0	\times	1	128	1	127	1	257
18	3	\times	3	64	2	63	1	65
19	-	-	2	\times	3	\times	-	-
20	10	16	12	16	10	15	10	17
21	2	\times	1	\times	2	\times	0	\times

Table 3.9.2. Cassaletto, Picket and Rice (1969) Test Integrals Set.

Integral	S_A	S_N	L_A	L_N	P_A	P_N	C_A	C_N
1	14	3	14	4	14	3	14	3
2	14	3	14	4	14	2	14	3
3	14	3	14	4	14	3	14	3
4	14	3	14	4	14	3	14	3
5	7	33	14	4	14	3	14	5
6	8	33	14	4	14	3	14	5
7	7	65	14	4	14	7	14	9
8	7	65	14	4	14	7	14	9
9	6	×	14	8	14	7	14	9
10	6	×	14	8	14	7	14	9
11	6	×	14	8	14	7	14	17
12	6	×	14	8	14	7	14	17
13	6	×	14	8	14	15	14	17
14	7	×	14	8	14	15	14	17
15	7	×	14	8	14	15	14	17
16	7	×	14	8	14	15	14	17
17	6	×	14	8	14	15	14	17
18	7	×	14	8	14	15	14	17
19	6	×	14	8	14	15	14	17
20	6	×	14	16	14	15	14	17
21	8	65	14	4	14	7	14	9
22	5	×	14	8	14	7	14	17
23	7	65	14	8	14	7	14	9
24	9	33	14	8	14	7	14	9
25	11	17	14	8	14	15	14	17
26	10	17	1	×	2	255	2	257
27	6	×	14	16	14	15	12	17
28	9	33	14	8	14	7	14	9
29	0	×	0	128	0	127	0	129
30	0	×	0	×	0	255	0	513
31	0	×	0	×	0	255	0	×
32	7	×	14	8	14	7	14	9
33	7	65	12	32	10	15	9	33
34	0	×	0	×	0	255	0	513
35	7	65	14	8	14	15	14	17
36	3	×	4	×	4	255	4	×
37	2	×	3	×	4	×	3	×
38	2	×	3	×	4	×	3	×
39	1	×	3	×	4	×	2	×
40	3	×	2	×	1	×	1	×
41	5	×	7	64	8	63	7	65
42	5	×	3	×	3	×	3	×
43	6	×	9	32	9	31	9	33
44	4	×	4	×	3	×	3	×
45	2	×	14	4	3	×	3	×
46	14	3	14	4	14	3	14	3
47	2	×	2	×	2	×	2	×
48	0	×	0	×	1	×	2	×
49	6	×	14	4	14	3	14	5
50	14	3	14	4	14	3	14	3

4

Improper Integrals

Improper integrals are such that their range or integrands are unbounded. They are defined as the limits of certain proper integrals. Thus, an improper integral over the interval $[0, \infty)$ is defined as $\int_0^\infty f(x) dx = \lim_{R \rightarrow \infty} \int_0^R f(x) dx$ whenever the limit exists. Improper integrals over $[a, \infty)$, $(-\infty, a]$ are similarly defined. Improper integrals over the interval $(-\infty, \infty)$ are defined in two ways: First, there is the usual definition: $\int_{-\infty}^\infty f(x) dx = \int_{-\infty}^0 f(x) dx + \int_0^\infty f(x) dx$. Then, there is the other definition: $\int_{-\infty}^\infty f(x) dx = \lim_{R \rightarrow \infty} \int_{-R}^R f(x) dx$, provided both limits exist. This definition is also known as *Cauchy's principal value* (or p.v.) of the integral, denoted by $\oint_{-\infty}^\infty f(x) dx$. A common p.v. integral is the Hilbert transform $\oint_A^b \frac{f(t)}{t-x} dt$, where $-\infty \leq a < b \leq \infty$, and $a < x < b$. A sufficient condition for the Hilbert transform to exist over a finite interval $[a, b]$ is that $f(t)$ satisfy a *Lipschitz* or *Hölder* condition in $[a, b]$; i.e., there are constants $A > 0$ and $0 < \alpha \leq 1$ such that for any two points $t_1, t_2 \in [a, b]$ we have $|f(t_1) - f(t_2)| \leq A |t_1 - t_2|^\alpha$. Cauchy's p.v. integrals are discussed in [Chapter 6](#).

4.1. Infinite Range Integrals

We discuss some methods and quadrature rules for computation of infinite range integrals.

4.1.1. Truncation Method. The technique of truncating the infinite interval of integration is discussed, and the Riemann method is used on the truncated interval,

which is valid if the integrand decays rapidly. We consider infinite range integrals of the form

$$I_1 = \int_a^\infty w(x) f(x) dx, \quad I_2 = \int_{-\infty}^\infty w(x) f(x) dx. \tag{4.1.1}$$

If the product $w(x) f(x)$ tends to zero rapidly near the ‘infinite’ endpoint(s), then, by the Riemann sum method, we have

$$I_1 = \lim_{R \rightarrow \infty} \int_a^R w(x) f(x) dx = \lim_{R \rightarrow \infty} I_1(R), \tag{4.1.2}$$

$$I_2 = \lim_{R \rightarrow \infty} \int_{-R}^R w(x) f(x) dx = \lim_{R \rightarrow \infty} I_2(R), \tag{4.1.3}$$

Thus, we can truncate the range only if the product $w(x)f(x)$ decays rapidly for large $|x|$.

EXAMPLE 4.1.1. (Delves and Mohamed 1985, p. 39) Compute

$$\begin{aligned} I_1 &= \int_0^\infty e^x \sin x \, dx = 0.5, \\ I_2 &= \int_0^\infty \frac{dx}{x^2 + 100} \, dx = \frac{\pi}{2} = 0.157079632. \end{aligned}$$

We truncate the upper limit at a value $R > 0$, and for fixed R we use an N -point Gaussian rule. The results are given in Table 4.1.1. It is found that this rule gives good results for $I_1(f)$ at a small value of N (at $R = 15$ and $N = 16$), but for $I_2(f)$ it is not that satisfactory even for $R = 200$ at $N = 32$. Also see [Example 4.1.6](#).

Table 4.1.1. Truncation Method.

<i>R</i>	<i>N</i>	<i>I</i> ₁ (<i>R</i>)	<i>R</i>	<i>N</i>	<i>I</i> ₂ (<i>R</i>)
5.0	8	0.502275	5.0	4	0.046356
10.0	8	0.500314	10.0	4	0.078540
15.0	16	0.500000	15.0	4	0.098279
			20.0	8	0.110715
			25.0	8	0.119029
			50.0	16	0.137340
			100.0	16	0.147113
			200.0	32	0.152084 ■

4.1.2. Gaussian Rules. Assuming that the integrals over infinite intervals are convergent, there are two major methods for their computation: (i) If the integrand

is such that the integral remains bounded in magnitude from some finite value to infinity by some constant $\varepsilon > 0$, we use a quadrature (like the Gauss-Legendre rule) for the remaining finite interval; and (ii) we develop a quadrature rule especially for the infinite interval. The first method has been considered before and does not need any further consideration. For the second method where we compute integrals over infinite and semi-infinite intervals, we will use such a weight function $w(x)$ that would maintain the convergence of the integral of $w(x)f(x)$, where $f(x)$ is a polynomial of arbitrary degree.

GAUSS-LAGUERRE RULE (§3.2.3). If the interval is semi-infinite, say (a, ∞) , we will take $a = 0$ for convenience, and choose the weight function $w(x) = e^{-x}$. This demands that the sequence of polynomials that we use must be orthogonal over $(0, \infty)$ with respect to e^{-x} . The polynomials that meet this requirement are the Laguerre polynomials $L_n(x)$ of degree n , with the leading coefficient $A_n = (-1)^n$. Thus, the *Gauss-Laguerre quadrature rule* is

$$\int_0^\infty e^{-x} f(x) dx = \sum_{i=1}^n w_i f(x_i) + E_n, \quad (4.1.4)$$

where x_i are the zeros of $L_n(x)$, and

$$w_i = \frac{(n!)^2}{L_{n+1}(x_i) L'_n(x_i)}, \quad (4.1.5)$$

$$E_n = \frac{(n!)^2}{(2n)!} f^{(2n)}(\xi), \quad \text{for } \xi \in (0, \infty). \quad (4.1.6)$$

Note that $\int_0^\infty e^{-x} L_n^2(x) dx = (n!)^2 = \gamma_n$. Some of the weights w_i and nodes x_i for the Gauss-Laguerre rule are given in [Table A.7](#).

EXAMPLE 4.1.2. Compute $I = \int_0^\infty e^{-x} x^3 dx = 6$ by the Gauss-Laguerre rule with $N = 2$ which is exact for all polynomials of degree at most 3. For $N = 2$ we have $L_2(x) = x^2 - 4x + 2$ and its zeros are at $\xi_{1,2} = 2 \pm \sqrt{2}$. The weights are given by $w_j = \frac{(2!)^2}{\xi_j [L'_2(\xi_j)]^2}$, $j = 1, 2$ (see §3.3.3). Thus, $w_{1,2} = \frac{1}{4} (2 \mp \sqrt{2})$. Then the Gauss-Laguerre rule gives

$$I = \frac{1}{4} (2 - \sqrt{2}) (2 + \sqrt{2})^3 + \frac{1}{4} (2 + \sqrt{2}) (2 - \sqrt{2})^3 = 6,$$

which is the exact value of If . ■

EXAMPLE 4.1.3. Compute $I = \int_1^\infty e^{-x} x^3 dx$ by the Gauss-Laguerre rule with $N = 2$. Using the values of ξ_j and w_j from Example 4.1.2 we find that

$$I = \frac{1}{e} \left[\frac{1}{4} (2 - \sqrt{2}) (2 + \sqrt{2})^3 + \frac{1}{4} (2 + \sqrt{2}) (2 - \sqrt{2})^3 \right] = \frac{16}{e},$$

which is the exact value of If . ■

GAUSS-HERMITE RULE (§3.2.4). If the interval is $(-\infty, \infty)$, we choose the weight function $w(x) = e^{-x^2}$. Then the Hermite polynomials $H_n(x)$ of degree n , with the leading coefficient $A_n = 2^n$, are orthogonal to e^{-x^2} over the interval $(-\infty, \infty)$. Thus, the *Gauss-Hermite quadrature rule* is

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \sum_{i=1}^n w_i f(x_i) + E_n, \quad (4.1.7)$$

where x_i are the zeros of $H_n(x)$, and the weights are given by

$$w_i = -\frac{2^{n+1} n! \sqrt{\pi}}{H_{n+1}(x_i) H'_n(x_i)}, \quad (4.1.8)$$

$$E_n = \frac{n! \sqrt{\pi}}{2^n (2n)!} f^{(2n)}(\xi), \quad \text{for } \xi \in (-\infty, \infty). \quad (4.1.9)$$

Note that $\int_0^{\infty} e^{-x^2} H_n^2(x) dx = \sqrt{\pi} 2^n n! = \gamma_n$. Some of the weights w_i and nodes x_i for the Gauss-Hermite rule are given in [Table A.8](#).

EXAMPLE 4.1.4. Compute

$$I = \int_{-\infty}^{\infty} e^{-x^2} x^4 dx = \frac{3\sqrt{\pi}}{4},$$

using Gauss-Hermite rule with $N = 3$. Here, $H_3(x) = 4x(x^2 - 3)$ and its zeros are $\xi_1 = 0$, and $\xi_{2,3} = \pm\sqrt{3/2}$. The weight are

$$w_j = \frac{2^4 3! \sqrt{\pi}}{[H'_3(\xi_j)]^2}, \quad j = 1, 2, 3.$$

Thus, $w_1 = \frac{2\sqrt{\pi}}{3}$, and $w_2 = \frac{\sqrt{\pi}}{6} = w_3$. Hence,

$$I \approx \frac{2\sqrt{\pi}}{3} \cdot 0 + \frac{\sqrt{\pi}}{6} \left(-\sqrt{3/2}\right)^4 + \frac{\sqrt{\pi}}{6} \left(\sqrt{3/2}\right)^4 = \frac{3\sqrt{\pi}}{4},$$

which is the exact value of If . ■

EXAMPLE 4.1.5. Compute $\int_0^{\infty} x^7 e^{-x} dx$, using $n = 3$ in the rule (4.1.4). From [Table A.8](#) we find that

$$\begin{aligned} \int_0^{\infty} x^7 e^{-x} dx &\approx (0.711093) (0.415775)^7 + (0.278518) (2.294280)^7 \\ &\quad + (0.010389) (6.289945)^7 = 4139.9. \end{aligned}$$

The exact value of the integral is $7! = 5040$. The error is $E_3 = \frac{(3!)^2}{6!} 71\xi = 252\xi$, where $\xi \in (0, \infty)$, so it cannot be bounded. But the huge error is not surprising. This rule should be avoided if the derivative in the error term cannot be bounded. The better method appears to be the Gauss-Legendre rule. Note in passing that the Gauss-Laguerre rule for $n = 4$ gives a little better result as can be seen from the following computation:

$$\int_0^\infty x^7 e^{-x} dx \approx (0.603154)(0.322548)^7 + (0.357419)(1.745761)^7 \\ + (0.003612)(7.085810)^7 + (0.000023)(12.640801)^7 = 4443.3.$$

But with $n = 5$, the computed value

$$(0.521756)(0.263560)^7 + (398667)(1.413403)^7 \\ + (0.075942)(3.596426)^7 + (0.003612)(7.085810)^7 + (0.000023)(12.640801)^7 \\ = 4.49735386 \times 10^6,$$

is way off the exact value. ■

The midpoint and trapezoidal rules are useful in computing with high accuracy integrals of the form $\int_{-\infty}^\infty e^{-t^2} f(t) dt$ and other integrals that decay rapidly for large $|t|$ (see Goodwin 1949). These rules are used to derive quadrature formulas with exponential convergence for finite and semi-infinite intervals.

EXAMPLE 4.1.6. To compare the accuracy of the midpoint and Gauss-Hermite quadrature Squire (1987) considers the integral

$$\int_{-\infty}^\infty e^{-t^2} \cos(2kt) dt = \sqrt{\pi} e^{-k^2}. \quad (4.1.10)$$

Let

$$V(x, y) = \frac{y}{\pi} \int_{-\infty}^\infty \frac{e^{-t^2}}{(x-t)^2 + y^2} dt = \Re \left\{ \frac{i}{\pi} \int_{-\infty}^\infty \frac{e^{-t^2}}{z-t} dt \right\}, \quad (4.1.11)$$

denote the Voigt function which is used in spectroscopy. Note that the integral $\Im \left\{ \frac{i}{\pi} \int_{-\infty}^\infty \frac{e^{-t^2}}{z-t} dt \right\}$ is known as Dawson integral. Humlecek (1979) has found that the integrals in (4.1.10) and (4.1.11) are difficult to compute for small x and y because of the poles at $t = x \pm iy$. Squire (1987) uses the quadrature formula

$$\int_{-\infty}^\infty \frac{e^{-t^2}}{z-t} dt = \sum_{k=1}^N \frac{A_k}{z-t_k},$$

where A_k and t_k denote the weights and nodes, respectively. Then the formula

$$\int_{-\infty}^\infty e^{-t^2} \cos(2kt) dt \approx e^{-k^2} \sum_{k=1}^N A_k \frac{(-\sin(2kt_k) + i \cos(2kt_k))}{(x+t_k) + i(y+k)}$$

becomes useful in computation if k is chosen such that the quadrature rule gives desired accuracy for the integral (4.1.10). Squire finds that for 12 nodes the midpoint rule computes (4.1.10) more accurately than Gauss-Hermite rule, and his method gives accurate results for $z = 0$. ■

4.1.3. Mapped Finite Range Rules. The weight functions for both Gauss-Laguerre and Gauss-Hermite quadrature rules decay exponentially. They appear to be suitable for the first integral in Examples 4.1.1, 4.1.2 and 4.1.3 but not for Example 4.1.5. Other infinite range rules can be produced by using the method of variable transformations. This is done in two ways: Either we map the integral $I_a^b(f)$ onto $I_{-1}^1(f)$, or we map a rule defined on $[-1, 1]$ onto the required interval of integration. We will discuss the latter method because it tells us more about the types of integrand for which the particular mapping is appropriate. For example, consider the integral

$$I(f) = \int_a^\infty f(x) dx. \quad (4.1.12)$$

If we use the transformation $x = \frac{2(a + \alpha)}{u + 1} - \alpha$, where α is arbitrary but such that $a + \alpha > 0$, then we find that

$$I(f) = 2(a + \alpha) \int_{-1}^1 \frac{F(u)}{(u + 1)^2} du, \quad (4.1.13)$$

where $F(u) = f(x)$. Let $\{\xi_j, w_j\}$, $j = 1, \dots, N$, be the nodes and weights of an N -point Gauss-Legendre rule. Then we have the rule

$$If \approx I_N = 2(a + \alpha) \sum_{j=1}^N w_j \frac{F(\xi_j)}{(\xi_j + 1)^2}, \quad (4.1.14)$$

which is exact if $\frac{F(u)}{(u + 1)^2}$ is a polynomial of degree $\leq 2N - 1$, i.e., for the class of functions $F(u) = (u + 1)^k$, $k = 2, 3, \dots, 2N + 1$. For this class the Gaussian rule, known as the *Gauss-Rational rule*, becomes

$$\int_a^\infty f(x) dx = \sum_{j=1}^N w'_j \frac{F(\xi'_j)}{(\xi'_j + 1)^2}, \quad (4.1.15)$$

where

$$\xi'_j = \frac{2(a + \alpha)}{\xi_j + 1}, \quad w'_j = \frac{2(a + \alpha) w_j}{(\xi_j + 1)^2}, \quad (4.1.16)$$

ξ_j and w_j being the Gauss-Legendre nodes and weights. This rule is better suited for the second integrand in Example 4.1.1, which are known as ‘long-tailed’ integrands.

EXAMPLE 4.1.7. (Delves and Mohamed 1985, p. 43) Compute the second integral in Example 4.1.1 by the Gauss-rational rule. The results of the Gauss-Laguerre rule with different values of the parameter α are given in Table 4.1.4. The best results are obtained for $N = 48$ and $\alpha = 0.05$ which give an accuracy of about 2×10^{-4} . The results obtained from the Gauss-rational rule are compared with the Gauss-Laguerre rule for $a = 0$ and values of α as shown in Table 4.1.5.

Table 4.1.4. Gauss-Laguerre Rule with different values of α .

N	$\alpha = 1.0$	$\alpha = 0.5$	$\alpha = 0.2$	$\alpha = 0.1$	$\alpha = 0.05$
2	0.0551436	0.0909624	0.1274653	0.1493257	0.1479445
4	0.0927649	0.1215651	0.1423088	0.1501190	0.1610400
8	0.1228893	0.1394927	0.1499906	0.1533760	0.1561286
16	0.1401240	0.1485416	0.1536576	0.1553738	0.1560471
32	0.1487845	0.1529250	0.1554170	0.1562483	0.1566703
48	0.1516143	0.1543449	0.1559855	0.1565326	0.1568056

The exact value is 0.157079632.

Table 4.1.5. Gauss-Laguerre and Gauss-Rational Rules.

N	Gauss-Laguerre ($\alpha = 0.2$)	Gauss-Rational ($\alpha = 10$)
2	0.1274653	0.1500000
4	0.1423088	0.1568627
8	0.1499906	0.1570794
16	0.1536576	0.1570796
32	0.1554170	
48	0.1559855	■

4.2. Improper Integrals

The formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx \approx h \sum_{n=-\infty}^{+\infty} e^{-n^2 h^2} \quad (4.2.1)$$

is accurate even for large values of h ; for example, for $h = 1$, the error is one unit in the fourth decimal place, i.e., it is of the order 10^{-4} . The quadrature formula using central differences for integration over one subinterval is

$$\int_a^{a+h} f(x) dx \approx \frac{h}{2} [f(a) + f(a+h)] + h \sum_{k=1}^{\infty} \frac{B_{2k}^{(2k)}(k)}{(2k)!} \mu \delta^{2k-1} [f(a+h) - f(a)], \quad (4.2.2)$$

where $B_{2k}^{(2k)}(k)$ denote the Bernoulli numbers (see §2.2.2). By adding such formulas

over m subintervals, we get

$$\begin{aligned} \int_a^{a+mh} f(x) dx &\approx h \left[\frac{1}{2} f(a) + f(a+h) + \cdots + \frac{1}{2} f(a+mh) \right] \\ &\quad + h \sum_{k=1}^{\infty} \frac{B_{2k}^{(2k)}(k)}{(2k)!} \mu \delta^{2k-1} [f(a+mh) - f(a)]. \end{aligned} \quad (4.2.3)$$

Now, the function e^{-x^2} and its differences approach zero rapidly as $x \rightarrow \pm\infty$, while the series (4.2.2) does not converge but is asymptotic, and the error caused by the approximation (4.2.1) can be obtained from the magnitude of the remainder term. If $n-1$ terms are taken in the infinite series (4.2.2), the remainder is given by

$$R_n = h^{2n+1} \frac{B_{2k}^{(2k)}(k)}{(2k)!} f^{(2n)}(\xi), \quad a-nh < \xi < a+nh. \quad (4.2.4)$$

For $f(x) = e^{-x^2}$ we have $f^{(2n)}(\xi) = \frac{d^{2n}}{d\xi^{2n}} e^{-\xi^2} = e^{-\xi^2} H_{2n}(\xi)$, where $H_{2n}(\xi)$ are the Hermite polynomials. Thus, for large n we have

$$f^{(2n)}(\xi) \sim (-1)^n 2^{2n+1/2} \left(\frac{n}{e}\right)^n e^{-\xi^2/2} \cos 2\xi\sqrt{n}, \quad (4.2.5)$$

$$\frac{B_{2n}^{(2n)}(n)}{(2n)!} \sim (-1)^{n-1} n^{-3/2} \pi^{-5/2} 2^{-2n+1}. \quad (4.2.6)$$

Substituting (4.2.5) and (4.2.6) into (4.2.4) we get

$$R_n \sim -\frac{2^{3/2} h}{n^{3/2} \pi^{5/2}} \left(\frac{n h^2}{e}\right)^n e^{-\xi^2/2} \cos 2\xi\sqrt{n}, \quad (4.2.7)$$

which implies that even if h is taken small, R_n will eventually increase without limit. Thus we have the quadrature rule

$$\int_{-\infty}^{\infty} f(x) e^{-x^2} dx = h \sum_{n=-\infty}^{\infty} f(nh) e^{-n^2 h^2} - E(h). \quad (4.2.8)$$

Without loss of generality, we take $f(x)$ to be an even function. Then integrating $\frac{f(x) e^{-x^2}}{1 - e^{-2i\pi x/h}}$ around a rectangular contour with vertices at $\pm\infty \pm \frac{i\pi}{h}$, we find that

$$\left(\int_{-\infty-i\pi/h}^{+\infty-i\pi/h} + \int_{+\infty+i\pi/h}^{-\infty+i\pi/h} \right) \frac{f(x) e^{-x^2}}{1 - e^{-2i\pi x/h}} dx = h \sum_{n=-\infty}^{\infty} f(nh) e^{-n^2 h^2}. \quad (4.2.9)$$

Hence,

$$\begin{aligned}
 h \sum_{n=-\infty}^{\infty} f(nh) e^{-n^2 h^2} &= \int_{-\infty-i\pi/h}^{\infty-i\pi/h} f(x) e^{-x^2} dx \\
 &= \int_{-\infty-i\pi/h}^{+\infty-i\pi/h} \frac{f(x) e^{-x^2} e^{-2\pi i x/h}}{1 - e^{-2\pi i x/h}} dx + \int_{\infty+i\pi/h}^{-\infty+i\pi/h} \frac{f(x) e^{-x^2}}{1 - e^{-2\pi i x/h}} dx \\
 &= 2 \int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x) e^{-x^2}}{e^{2\pi i x/h} - 1} dx, \quad \text{since } f(x) \text{ is even.}
 \end{aligned} \tag{4.2.10}$$

If $f(x)$ has no poles between the real axis and the lines $x = \pm i\pi/h$, then

$$E(h) = 2 e^{-\pi^2/h^2} \int_{-\infty}^{\infty} f(u - i\pi/h) e^{-u^2} du. \tag{4.2.11}$$

For example, if $f(x) \equiv 1$, then $E(h) = 2\sqrt{\pi} e^{-\pi^2/h^2}$. Note that $E(h) \approx 1.8 \times 10^{-4}$ for $h = 1$, and $E(h) \approx 2.5 \times 10^{-17}$ for $h = 0.5$. A simpler expression for error is

$$E(h) = 2\sqrt{\pi} e^{-\pi^2/h^2} f(i\pi/h), \tag{4.2.12}$$

although this error estimate is not very effective if $f(x) \rightarrow \infty$ rapidly as $x \rightarrow \infty$.

For example, if $f(x) = x^2$, then from (4.2.12) we get $E(h) = -2\sqrt{\pi} \frac{\pi^2}{h^2} e^{-\pi^2/h^2}$

instead of the accurate error bound $E(h) = -2\sqrt{\pi} \left(\frac{\pi^2}{h^2} - \frac{1}{2} \right) e^{-\pi^2/h^2}$. If $f(x)$ is of the form $f(x) = \phi(x) \cosh kx$, then (4.2.12) is replaced by

$$E(h) \sim 2\sqrt{\pi} e^{-\pi^2/h^2 + k^2/4} \phi(i\pi h). \tag{4.2.13}$$

EXAMPLES 4.2.1. Some other examples are:

1. For $\int_{-\infty}^{\infty} \cos x e^{-x^2} dx = \sqrt{\pi} e^{-1/4}$, the error bound is

$$E(h) \sim 2\sqrt{\pi} e^{-\pi^2/h^2} \cos(\pi/h) \sim \sqrt{\pi} e^{\pi/h - \pi^2/h^2}.$$

2. For $\int_{-\infty}^{\infty} x^2 \cos x e^{-x^2} dx = \frac{1}{4} \sqrt{\pi} e^{-1/4}$, the error bound is

$$E(h) \sim \sqrt{\pi} \left(\frac{\pi^2}{h^2} \right) e^{\pi/h - \pi^2/h^2}.$$

3. For $\int_{-\infty}^{\infty} J_0(x) e^{-x^2} dx = \sqrt{\pi} e^{-1/8} I_0(1/8)$, the error bound is

$$E(h) \sim 2\sqrt{\pi} I_0(\pi/h) e^{-\pi^2/h^2} \sim \sqrt{\frac{2h}{\pi}} e^{\pi/h - \pi^2/h^2}.$$

4. For $\frac{1}{\sqrt{\pi}} \int_0^\infty e^{-u^2/4} \cos xu J_0(yu) du$, the error bound from (4.2.12) is

$$E(h) \sim \frac{1}{2\pi} \left(\frac{h}{y}\right)^{1/2} e^{2\pi(x+y)/h - \pi^2/h^2}.$$

5. For $\int_0^\infty (x^2 - \frac{1}{2}) e^{-x^2} [Y_0(|a+bx|) + Y_0(|a-bx|)] dx$, the error bound from (4.2.12) is

$$E(h) \sim \sqrt{\pi} \left(\frac{\pi^2}{h^2} + \frac{1}{2}\right) e^{2\pi/h - \pi^2/h^2}.$$

Note that in all these five examples, the exact value of the integral is known. ■

We start with the Euler-Maclaurin summation formula (2.2.8) and obtain

$$\begin{aligned} \sum_{n=0}^{N-1} h f(n\delta) &= \int_0^N h f(x) dx - \frac{h}{2} [f(nh) - f(0)] \\ &\quad + \sum_{k=1}^{\infty} \frac{(-1)^{k+1} B_k}{(2k)!} h^{2k} \left(\frac{d}{dx}\right)^{2k-1} f \Big|_{x=0}^{x=nh}, \end{aligned} \quad (4.2.14)$$

where B_k are the Bernoulli numbers. This formula reduces to the trapezoidal rule if the term with one-half the endpoints is included; then the error is of the order h^2 . It also reduces to the Simpson's rule if we add two such series at alternate nodes so as to cancel out the h^2 terms; then the error is of the order h^4 . Moreover, if the first derivative of f vanishes at the endpoints of the integration, then the sum (4.2.14) differs from the integral in order h^{p+2} , where $p \geq 1$ is an integer. Thus, we can take

$$I(f) = \int_{-\infty}^{\infty} f(x) dx \approx \sum_{n=-\infty}^{\infty} h f(nh). \quad (4.2.15)$$

We assume that the integrand $f(x)$ goes to zero at the endpoints fast enough so that both the integral and the sum converge, and we assume that f is an analytic function on the real axis on which we are integrating and also within the strip $|\Im\{x\}| \leq a$ in the complex z -plane. Now, consider the integral representation

$$\Sigma = \oint \frac{f(x) dx}{e^{2\pi ix/h} - 1} \equiv \Sigma_+ + \Sigma_-, \quad (4.2.16)$$

where

$$\begin{aligned} \Sigma_- &\equiv \int_{-\infty-i\varepsilon}^{+\infty-i\varepsilon} \frac{f(x) dx}{e^{2\pi ix/h} - 1}, \\ \Sigma_+ &\equiv \int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} \frac{f(x) dx}{e^{2\pi ix/h} - 1} = \int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} f(x) \left[1 + \frac{1}{e^{-2\pi ix/h} - 1}\right] dx. \end{aligned} \quad (4.2.17)$$

Then $\sum = I(f) + E$, where the error E is given by

$$\begin{aligned} E &= \int_{-\infty-i\varepsilon}^{+\infty-i\varepsilon} \frac{f(x) dx}{e^{2\pi i x/h} - 1} + \int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} \frac{f(x) dx}{e^{-2\pi i x/h} - 1} \\ &\sim e^{-A} \left[\int_{-\infty}^{\infty} f(x - ia) e^{-2\pi i x/h} dx + \int_{-\infty}^{\infty} f(x + ia) e^{2\pi i x/h} dx \right] \\ &= o\left(e^{-2\pi a/h}\right), \end{aligned} \quad (4.2.18)$$

which shows that the error decreases faster than any power of h . Note that halving the interval *doubles* the number of correct decimal digits in the result.

EXAMPLE 4.2.2. Consider $f(x) = \frac{1}{e^x + e^{-x}}$. This integrand has singularities at $x = \pm i\pi/2$, so $a = \pi/a$, and $E \approx e^{-\pi\sqrt{N/2}}$. This is rapid convergence. For $N = 10$ the error is about 10^{-3} , and for $N = 100$ it is about 10^{-10} . ■

EXAMPLE 4.2.3. Consider $f(x) = \frac{1}{1+x^2}$. The value of $a = 1$, and $E \approx e^{-2\pi/h}$. ■

4.2.1. Method of Variable Transformations. This method is known to compute improper integrals provided a proper choice of the mapping function which is ingeniously obtained for each integral on a case-by-case basis. A general method for variable transformations is given by Schwartz (1969), which is applicable to a large class of improper integrals. In this method the mapping function is chosen such that the singularities of the integrand are moved to infinity; this changes the improper integral into a convergent infinite integral which can be computed by the trapezoidal rule with an equal step size h . The application of such a trapezoidal rule over the interval $(-\infty, \infty)$ provides an unusually high accuracy provided the integrand is analytic over this interval except the endpoints (see Goodwin 1949).

We will derive quadrature formulas for the computation of improper integrals of the form (i) $\int_a^b f(x) (1-x)^{-\alpha} (1+x)^{-\beta} dx$, $\alpha, \beta < 1$, and (ii) $\int_{-\infty}^{\infty} f(x) dx$, where for integrals of type (i) we use variable transformations like $x = \tanh u$ and $x = \operatorname{erf} u$, followed by the trapezoidal rule, whereas for integrals of the type (ii) we use the variable transformations like $x = \sinh u$ and $x = \tan u$, followed by the trapezoidal rule. The error bounds for these quadrature formulas are obtained by the method of contour integration.

Let $I_a^b(f) = \int_a^b f(x) dx$, where a and b may be infinite. It is assumed that $f(x)$ is analytic in a certain domain that includes the line segment (a, b) . The method of variable transformation is as follows: We make a change of variables by setting $x = \phi(u)$, where $\phi(u)$ is analytic in a certain domain and maps univalently the line segment $c \leq u \leq d$ onto $a \leq x \leq b$, where c and d may be infinite. Then the

transformed integral is

$$I = \int_c^d g(u) du, \quad \text{where } g(u) = f(\phi(u)) \phi'(u). \quad (4.2.19)$$

The function $g(u)$ is also analytic in a certain domain that includes (c, d) . Then we apply any quadrature rule to (4.2.19), which gives

$$\begin{aligned} I &\approx I_w = \sum_j w_j g(x_j) \\ &= \sum_j w_j \phi'(x_j) f(\phi(x_j)) = \sum_j \omega_j f(\xi_j), \end{aligned} \quad (4.2.20)$$

where $\xi_j = \phi(x_j)$ are the nodes and $\omega_j = w_j \phi'(x_j)$ are the weights of the new quadrature rule. The error in formula (4.2.20) is $E = \int_c^d g(u) du - \sum_j w_j g(x_j)$, which is written in the contour integration form obtained by substituting Cauchy's integral representation for $g(u)$ as

$$E = \frac{1}{2i\pi} \oint_{\hat{C}} \hat{\phi}(w) g(w) dw, \quad (4.2.21)$$

where

$$\hat{\phi}(w) = \int_c^d \frac{du}{w-u} - \sum_j \frac{w_j}{w-x_j}. \quad (4.2.22)$$

The function $\hat{\phi}(w)$ which is defined in the complex w -plane is known as the *characteristic function* of the quadrature error E . The contour \hat{C} is traversed counter-clockwise and it encloses the line segment (c, d) . The contour integration in (4.2.22) is evaluated by the saddle point method (see, e.g., [Carrier et al. 1966](#), p. 258ff.) If we use the inverse transformation $z = \phi(w)$, then formula (4.2.22) yields another formula for the quadrature error:

$$E = \frac{1}{2i\pi} \oint_C \phi(z) f(z) dz, \quad (4.2.23)$$

where the function $\phi(z) = \hat{\phi}(w)$ is defined in the complex z -plane, and the path C is the inverse image of \hat{C} from the w -plane into the z -plane under the map $z = \phi(w)$. Note that formula (4.2.23) gives the quadrature error directly in terms of the given function $f(z)$. Thus, we can regard $\phi(z)$ as the characteristic function of the original formula (4.2.20) and choose between formula (4.2.22) and (4.2.23) according to convenience.

Now, we consider $I = \int_{-1}^1 f(x) dx$, where $f(x)$ may have singularities at one or both endpoints.

CASE 1. THE TANH-RULE. Let the mapping function be $x = \tanh u$. Then

$$I = \int_{-\infty}^{\infty} f(\tanh u) \operatorname{sech}^2(u) du,$$

which, after applying the trapezoidal rule with an equal mesh size, gives the quadrature formula

$$I_w = h \sum_{n=-\infty}^{\infty} f(\tanh nh) \operatorname{sech}^2(nh). \quad (4.2.24)$$

This formula is known as the *Tanh-Rule*. The error in (4.2.24) is given by

$$E = \frac{1}{2i\pi} \int_{\hat{C}} \hat{\phi}(w) f(\tanh w) \operatorname{sech}^2(w) dw, \quad (4.2.25)$$

where $\hat{\phi}(w)$ is given by (Takahasi and Mori 1971)

$$\hat{\phi}(w) = \begin{cases} \frac{-2i\pi}{1 - \exp(-2i\pi w/h)} \approx 2i\pi \exp(2i\pi w/h) & \text{if } \Im\{w\} > 0, \\ \frac{2i\pi}{1 - \exp(2i\pi w/h)} \approx -2i\pi \exp(-2i\pi w/h) & \text{if } \Im\{w\} < 0. \end{cases} \quad (4.2.26)$$

The contour \hat{C} consists of two lines which run along both sides of the real axis. The inverse characteristic function $\phi(z)$ in the z -plane is

$$\phi(z) = \hat{\phi}(\operatorname{arctanh} z) \approx \begin{cases} 2i\pi \left(\frac{1+z}{1-z} \right)^{i\pi/h} & \text{if } \Im\{z\} > 0, \\ -2i\pi \left(\frac{1+z}{1-z} \right)^{-i\pi/h} & \text{if } \Im\{z\} < 0, \end{cases} \quad (4.2.27)$$

which gives

$$E = \frac{1}{2i\pi} \int_C \phi(z) f(z) dz. \quad (4.2.28)$$

Note that since $\operatorname{arctanh} z$ is multiple-valued, each strip domain $\{w : -\pi/2 + m\pi < \Im\{w\} < \pi/2 + m\pi\}$, $m = 0, \pm 1, \pm 2, \dots$, is mapped onto the entire z -plane cut along $-\infty, -1$ and $(1, \infty)$. This means that the characteristic function $\phi(z)$, defined by (4.2.27), and the integrand in (4.2.28) should be defined on the Riemann surface such that the path C may also run outside the principal sheet. The contour $|\hat{\phi}(w)| = \varepsilon$ in the w -plane is approximately a pair of straight lines given by $\Im\{w\} = \pm \frac{h}{2\pi} \log \left(\frac{2\pi}{\varepsilon} \right)$, which implies that the contour $|\phi(z)| = \varepsilon$ is a pair of circular arcs $x^2 + (y \pm \cot 2c_0)^2 = \csc^2(2c_0)$, which meet at $z = \pm 1$, where $z = x + iy$, and $c_0 = \frac{h}{2\pi} \log \left(\frac{2\pi}{\varepsilon} \right)$.

According to Haber (1987) the tanh-rule approximates $I_{-1}^1(f)$ by

$$I_n(f) = h \sum_{j=-n}^n \frac{f(\tanh(jh/2))}{2 \cosh^2(jh/2)}, \quad h = h(n) \sim c n^{-1/2}. \quad (4.2.29)$$

The rule is very accurate, and its error is $O(e^{-c\sqrt{n}})$ for some $c > 0$, even when the integrand is unbounded at an endpoint of the interval of integration. Let Λ_d denote the region in the complex plane bounded by two circular arcs passing through $-$ and $+$, one arc in the plane $\Im\{z\} > 0$ and the other in $\Im\{z\} < 0$ such that each arc makes an angle d with the real x -axis at each point ± 1 . It is assumed that $d > 0$, f is analytic in Λ_d , and $\int_{\Gamma_n} |f|$ is bounded along some sequence of contours $\{\Gamma_n\}$ that approach $\partial\Lambda_d$, and $f(x) = O((1-x^2)^{\alpha-1})$ for some $\alpha > 0$ as $x \rightarrow \pm 1$ from inside $(-1, 1)$. Let us denote $\psi(x) = \tanh(x/2)$, and let $\phi(x) = \psi^{-1}(x) = \ln \frac{1+x}{1-x}$. Then

$$\begin{aligned} \int_{-1}^x f(t) dt &= h \sum_{k=-n}^n \psi'(kh) f(\psi(kh)) \left[\frac{1}{2} + \sigma\left(\frac{\phi(k)}{h} - k\right) \right] \\ &= O\left(e^{-\sqrt{\pi\alpha d n}}\right) \end{aligned} \quad (4.2.30)$$

uniformly in x , where $\sigma(x) = \frac{1}{\pi} \int_0^{\pi x} \frac{\sin t}{t} dt$ is a form of the sinc integral, and the quantity h depends on n such that $h(n) = \sqrt{\frac{\pi d}{\alpha n}} + \frac{\log n}{2\alpha n}$. The formula (4.2.30) needs a subroutine for computing the above sinc integral. An alternative formula is

$$\begin{aligned} \int_{-1}^x f(t) dt &= h \sum_{k=-n}^n \sum_{j=-n}^n \psi'(jh) f(\psi(jh)) \left[\frac{1}{2} + \sigma(k-j) \right] \operatorname{sinc}\left(\frac{\phi(x)}{h}\right) \\ &+ \left[h \sum_{j=-n}^n \psi'(jh) f(\psi(jh)) \right] \left[\eta(x) - \sum_{k=-n}^n \eta(\psi(kh)) \operatorname{sinc}\left(\frac{\phi(x)}{h}\right) \right] \\ &+ O\left(n e^{-\sqrt{\pi\alpha d n}}\right), \end{aligned} \quad (4.2.31)$$

where $\operatorname{sinc} x = \frac{\sin \pi x}{\pi x}$.

4.2.2. Types of Inherent Errors. In any quadrature rule that is obtained by a variable transformations method there is an inherent error which is unavoidable irrespective of the integrand, even when the integrand is a constant. To explain this situation, we will consider the integrand $f(x) = (1-x^2)^{-\alpha} f_1(x)$, $\alpha < 1$, where $f_1(x)$ is regular in a certain domain that includes the interval $[-1, 1]$. Then, we use (4.2.25) and deform the contour \hat{C} such that we can use the saddle point method. Since the integrand in (4.2.25) which is

$$F(w) = \phi(w) \frac{1}{\cosh^2 w} (1 - \tanh^2 w)^{-\alpha} f_1(\tanh w), \quad (4.2.32)$$

has singularities (poles or branch points) at $w = \pm i\pi/2$, we cannot move the path \hat{C} beyond these points. Also, for small values of h the variation of (4.2.32) is dominated by the rapid decay of $|\hat{\phi}(w)| \approx 2\pi \exp(-2\pi |\Im\{w\}|/h)$, i.e., for large $|\Im\{w\}|/h$, we should take the path \hat{C} close to these singularities, which gives a rough estimate for the error as

$$E(h) \approx |\hat{\phi}(\pm i\pi/2)| \approx 2\pi \exp(-\pi^2/h).$$

A precise error estimate by the saddle point method is $A \cdot 2\pi \exp(-\pi^2/h)$, where A is a factor of order 1 which depends on α . In the Tanh-rule, *this amount of error cannot be avoided* even when $\alpha = 0$, because the singularity is also contained in $\hat{\phi}(w)/\cosh^2 w$. We can expect a larger error if $f(z)$ has singularities outside the real axis.

Another type of inherent error is the truncation error E_T which is due to the replacement of the infinite sum $\sum_{n=-\infty}^{\infty}$ in formula (4.2.24) by a finite sum $\sum_{n=-N/2}^{N/2}$. For a given number of terms N , this error increases when h is decreased, which results in a decrease in $E(h) = 2\pi e^{-\pi^2/h}$. Thus, we can have an optimal value of h . For example, for the above function $f(x) = (1-x^2)^{-\alpha} f_1(x)$, $\alpha < 1$, the truncation error is given by $E_T \approx e^{-(1-\alpha)Nh}$. This leads to the optimal value of h as

$$h = \frac{\pi}{\sqrt{(1-\alpha)N}}.$$

Substituting this into the value of $E(h)$ we find that the dominating factor in the truncation error is

$$E_N \approx 2\pi e^{-\pi \sqrt{(1-\alpha)N}}, \quad (4.2.33)$$

where N is the number of nodes.

CASE 2. THE ERF-RULE. By taking the mapping function as $x = \operatorname{erf} u = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2} dt$, we get

$$I = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(\operatorname{erf} u) e^{-u^2} du. \quad (4.2.34)$$

which, after applying the trapezoidal rule with an equal mesh size, gives the quadrature formula

$$I_w = \frac{2h}{\sqrt{\pi}} \sum_{n=-\infty}^{\infty} f(\operatorname{erf} nh) e^{-n^2 h^2}. \quad (4.2.35)$$

This formula is known as the *Erf-Rule*. For this rule, the dominating factor in the truncation error is (see [Takahasi and Mori 1973](#))

$$E_N \approx 2\pi e^{-3.4 \sqrt[3]{(1-\alpha)N}}. \quad (4.2.36)$$

Thus, the Erf-rule is generally better than the Tanh-rule for integrands of the form $f(x) = (1 - x^2)^{-\alpha} f_1(x)$, where $f_1(z)$ is regular in the entire z -plane. The inherent error for this rule is of the order of $e^{-\pi^2/h^2}$ even when $\alpha = 0$.

CASE 3. THE IMT-RULE. This rule was developed by Iri, Moriguti and Takasawa (1970). It is obtained by the mapping function

$$x = \phi(u) = \frac{1}{Q} \int_{-1}^u \exp\left(-\frac{2}{1+t} - \frac{2}{1-t}\right) dt,$$

$$Q = \int_{-1}^1 \exp\left(-\frac{2}{1+t} - \frac{2}{1-t}\right) dt,$$

which maps the interval $(-1, 1)$ onto itself. Since all derivatives of $\phi(u)$ are zero at ± 1 , we apply to the transformed integral the trapezoidal rule with an equal mesh size of $h = 1/N$. The rule so obtained is known as the *ITM-Rule*. It is shown that for integrands that are of the same form as above, the inherent error for this rule is

$$E_N \approx 2\pi e^{-\sqrt{4\pi(1-\alpha)N}}, \quad (4.2.37)$$

This rule is as good as the Tanh-rule if the integrand $f(x)$ is regular except at $z = \pm 1$.

EXAMPLE 4.2.8. (Takahasi and Mori 1973) Consider

$$\int_{-1}^1 \frac{1}{(x-2)(x-1)^{1/4}(1+x)^{3/4}} dx = -1.949054456.$$

The errors in the above three quadrature rules are presented in Table 4.2.1. It is obvious from these results that the Erf-rule is superior to the other two rules for the same number of N , although the Tanh-rule is simpler to generate the sampling points and weights. In this example the error due to the simple pole at $x = 2$ is prominent as compared to that due to the singularities at $x = \pm 1$, except in the case of the Tanh-rule where both errors are of almost the same order of magnitude, since the segments of the real axis defined by $y = 0$, $|x| > 1$ are mapped onto the line $\Im\{w\} = \pi/2 + m\pi$ on which we have $|\hat{\phi}(w)| \approx 2\pi e^{-\pi^2/h}$. ■

EXAMPLE 4.2.9. (Takahasi and Mori 1973) Consider

$$\int_{-1}^1 \frac{\cos \pi x}{(1-x)^{1/2}} dx = -0.69049458699.$$

The errors in the above three quadrature rules are presented in Table 4.2.2. In this example the main source of error is the saddle point which is due to the fast growth of

$|\cos \pi w|$ and the rapid decay of $|\hat{\phi}(w)|$ along both directions of the imaginary axis. ■

Table 4.2.1. Errors in Tanh-Rule, Erf-Rule, and IMT-Rule.

N	Tanh-Rule (4.2.33)	Erf-Rule (4.2.36)	IMT-Rule (4.2.37)
5	1.87396(−1)	1.92742(−2)	1.19379(−1)
10	4.37433(−2)	6.43753(−4)	2.31187(−2)
50	9.42716(−5)	1.358082(−11)	2.2652(−5)
100	9.468868(−7)	1.908727(−18)	1.26041(−7)
150	2.774055(−8)	3.4156572(−24)	2.34692(−9)
200	1.414432(−9)	2.532692(−29)	8.16642(−11)
250	1.027632(−10)	4.883947(−34)	4.23737(−12)

Table 4.2.2. Errors in Tanh-Rule, Erf-Rule, and IMT-Rule.

N	Tanh-Rule (4.2.33)	Erf-Rule (4.2.36)	IMT-Rule (4.2.37)
5	4.3743(−2)	4.28295(−3)	2.31187(−2)
10	5.5891(−3)	5.5891(−5)	2.26818(−3)
50	9.46887(−7)	1.26148(−14)	1.26041(−7)
100	1.41443(−9)	2.93543(−23)	8.16642(−11)
150	9.60139(−12)	1.68487(−30)	2.92029(−13)
200	1.42697(−13)	5.79839(−37)	2.52837(−15)
250	3.49936(−15)	6.653(−43)	3.85184(−17)

Remark. While computing such integrals we must be careful not to lose significant digits due to cancellation as $x \rightarrow \pm 1$. In using the Tanh-rule or the Erf-rule, if possible, we should directly set $t = 1 - x = 1 - \tanh u = \frac{2e^{-2u}}{1 + e^{-2u}}$, or $t = 1 - x = 1 - \operatorname{erf} u$. There may also be possible underflow problems in computation.

4.3. Slowly Convergent Integrals

We will use the method of variable transformations to compute $I(f) = \int_{-\infty}^{\infty} f(x) dx$ when the integrands decay slowly as $x \rightarrow \infty$. An example of such integrands is $f(x) = (1 + x^2)^{-5/2}$. There are two cases:

CASE 1. SINH-RULE. We set $x = \sinh u$. Then

$$I(f) = \int_{-\infty}^{\infty} f(\sinh u) \cosh u \, du.$$

If we apply the trapezoidal rule with a uniform mesh size h , we obtain the quadrature

$$I_w = h \sum_{n=-\infty}^{\infty} f(\sinh nh) \cosh nh, \quad (4.3.1)$$

which is known as the *Sinh-Rule*. The error in this rule is given by

$$E = \frac{1}{2i\pi} \int_{\tilde{C}} \hat{\phi}(w) f(\sinh w) \cosh w \, dw, \quad (4.3.2)$$

where $\hat{\phi}(w)$ is defined by (4.2.26). The characteristic function $\phi(z)$ is defined in the z -plane by

$$\phi(z) = \hat{\phi}(\operatorname{arcsinh} z) \approx \begin{cases} 2i\pi (z + \sqrt{1+z^2})^{2i\pi/h} & \text{if } \Im\{z\} > 0, \\ -2i\pi (z + \sqrt{1+z^2})^{-2i\pi/h} & \text{if } \Im\{z\} < 0. \end{cases} \quad (4.3.3)$$

The contour map of $|\phi(z)|$ is obtained by mapping the straight lines $\Im\{w\} = \pm c_0$ onto the z -plane, where $c_0 = \frac{h}{2\pi} \log\left(\frac{2\pi}{\varepsilon}\right)$. This map is given by the family of confocal hyperbolas $-\frac{x^2}{\cos^2 c_0} + \frac{y^2}{\sin^2 c_0} = 1$ with foci at $z = \pm i$. The map $z = \sinh w$ takes each strip W_m defined in Case 1 of §4.2.1 onto the entire z -plane cut along $(-i\infty, -i) \cup (i, i\infty)$. On the principal sheet of the Riemann surface, $|\phi(z)|$ takes its minimum value which is approximately equal to $2\pi e^{-\pi^2/h}$ along the above cuts; $|\phi(z)|$ can never be smaller than this minimum value on the entire principal sheet.

In this case an integrand $f(z)$ must have at least one singularity in the entire z -plane either at a finite z or at infinity (where it must be an essential singularity since $f(z) \rightarrow 0$ as $x \rightarrow \pm\infty$). First, if there is a singularity at a finite z , then the contour C cannot go beyond this point; thus, the error is greater than the minimum value of $2\pi e^{-\pi^2/h}$. If there is an essential singularity at $z = \infty$ the modulus $|f(z)|$ must grow toward some direction $\arg\{z\} \neq 0, \pi$; thus, the contour C cannot be moved to infinity. In any case, there is an error of the order

$$E(h) \approx 2\pi e^{-\pi^2/h}. \quad (4.3.4)$$

The best situation is when the integrand has all its singularities on the cuts $(-i\infty, -i)$ and $(i, i\infty)$.

CASE 2. TAN-RULE. If the integrand $f(x)$ is regular at $x = \infty$, we use the transformation $x = \tan u$. Then we get

$$If = \int_{-\infty}^{\infty} f(x) dx = \int_{-\pi/2}^{\pi/2} f(\tan u) \sec^2 u du, \quad (4.3.5)$$

which is a finite integral with the integrand $f(\tan u) \sec^2 u$ which is a periodic function with period π regular along the real axis including the points $u = \pm\pi/2$, provided the original integral is convergent. We apply the trapezoidal rule with equally spaced nodes and obtain

$$I_w = h \sum_{n=-N/2}^{N/2-1} f(\tan nh) \operatorname{sech}^2 nh, \quad h = \pi/N, \text{ and } N \text{ even.} \quad (4.3.6)$$

This formula is known as the *Tan-Rule*. Its characteristic function $\hat{\phi}(w)$ is defined by (4.2.26), and the error is given by

$$E = \frac{1}{2i\pi} \int_{\tilde{C}} \hat{\phi}(w) f(\tan w) \operatorname{sech}^2 w dw, \quad (4.3.7)$$

where the contour \tilde{C} is a rectangle of width π which is the period of $\tan w$. The characteristic function $\phi(z)$ in the z -plane is given by

$$\phi(z) = \begin{cases} -\frac{2i\pi}{1 - \left(\frac{i-z}{i+z}\right)^{-N}} & \text{if } \Im\{z\} > 0, \\ \frac{2i\pi}{1 - \left(\frac{i-z}{i+z}\right)^N} & \text{if } \Im\{z\} < 0, \end{cases} \quad (4.3.8)$$

which is regular over each half-plane. The path of integration C is composed of two closed curves, each lying in the upper or lower half-plane and enclosing all the singularities in each half-plane, respectively. This contour C exists even when $\phi(z)$ is multiple-valued because $f(z)$ is regular at infinity. The map $z = \tan w$ takes the straight lines $|\hat{\phi}(w)| \approx \varepsilon$ in the w -plane into a family of circles $x^2 + (y - \coth 2c_0)^2 = \operatorname{csch}^2 2c_0$, where c_0 has the same value as before. Thus, the error becomes smaller as all singularities of $f(z)$ get closer to $\pm i$.

Assume that the integrand $f(x) \rightarrow 0$ as $x \rightarrow \infty$ in such a way that $\lim_{x \rightarrow \infty} f(x) x^\alpha = \text{const}$, where α is an integer ≥ 2 . Then the integrand in (4.3.5) vanishes at the end-points $u = \pm\pi/2$ whenever $\alpha > 2$. For $\alpha = 2$, this integrand remains finite, so we need to compute the value of $\lim_{x \rightarrow \infty} f(x) x^2$. But this leads to a serious problem if the function $g(u)$ is to be computed by using a computer. In such cases we use the midpoint rule

$$I_w = h \sum_{n=-N/2}^{N/2-1} f\left(\tan \frac{\pi}{N} \left(\frac{1}{2} + n\right)\right) \sec^2 \frac{\pi}{N} \left(\frac{1}{2} + n\right), \quad N \text{ even,} \quad (4.3.9)$$

since in this rule we do not need the function values at the end of the interval. This midpoint rule, however, is not recommended in automatic computer codes where the step size is halved repeatedly until the desired accuracy is achieved.

EXAMPLE 4.3.1. Consider

$$\int_{-\infty}^{\infty} \frac{dx}{1+x^4} = 2.221441469.$$

The errors are presented in Table 4.3.1.

Table 4.3.1. Errors in Tan-Rule and Sinh-Rule.

<i>N</i>	Tan-Rule (4.2.33)	Sinh-Rule (4.2.36)
5	4.3743(−2)	4.28295(−3)
10	5.5891(−3)	5.5891(−5)
50	9.46887(−7)	1.26148(−14)
100	1.41443(−9)	2.93543(−23)
150	9.60139(−12)	1.68487(−30)
200	1.42697(−13)	5.79839(−37)
250	3.49936(−15)	6.653(−43)

EXAMPLE 4.3.2. Consider

$$\int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{5/4}} = 2.39628,$$
$$\int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{-5/4}} = (1+x^2)^{1/4} \left(\frac{16}{21}x + \frac{2}{7}x^3 \right) + \frac{5}{21}x \, {}_2F_1\left(\frac{1}{2}, \frac{3}{4}, \frac{3}{2}; -x^2\right).$$

The errors are presented in Table 4.3.2 for the first integral; and in Table 4.3.3 for the second integral, for which we use the sin-rule by setting $x = \sin u$.

Table 4.3.2. Errors in Tan-Rule and Sinh-Rule.

<i>N</i>	Tanh-Rule (4.2.33)	Erf-Rule (4.2.36)	IMT-Rule (4.2.37)
5	4.3743(−2)	4.28295(−3)	2.31187(−2)
10	5.5891(−3)	5.5891(−5)	2.26818(−3)
50	9.46887(−7)	1.26148(−14)	1.26041(−7)
100	1.41443(−9)	2.93543(−23)	8.16642(−11)
150	9.60139(−12)	1.68487(−30)	2.92029(−13)
200	1.42697(−13)	5.79839(−37)	2.52837(−15)
250	3.49936(−15)	6.653(−43)	3.85184(−17)

Table 4.3.3. Errors in Sin-Rule.

N	Sin-Rule (4.2.36)
5	4.3743(−2)
10	5.5891(−3)
50	9.46887(−7)
100	1.41443(−9)
150	9.60139(−12)
200	1.42697(−13)
250	3.49936(−15)

4.4. Oscillatory Integrals

Consider the integrals of the form $I_0^\infty(wf) = \int_0^\infty w(x)f(x)dx$, where $w(x)$ is an oscillatory function. Numerical evaluation of such integrals involves mostly two cases: (i) $w(x) = \cos kx$ or $\sin kx$, and (ii) $w(x) = J_0(\omega x)$. The formulas developed by Filon (1928), Flinn (1960) and Clendenin (1966) are not applicable in such cases because of the infinite interval of integration.

4.4.1. Summation, then Integration. The earliest attempts to numerically integrate infinite range oscillatory functions were made by Hurwitz and Zweifel (1956), Hurwitz, Pfeifer and Zweifel (1959), Balbine and Franklin (1960) and Saenger (1964). These methods are based on partitioning the interval, followed by integrating between the successive zeros of $\sin kx$ or $\cos kx$, thus converting the infinite integral to summation. However, the problem with this method is that the resulting series converges very slowly. This slow convergence problem was corrected (i) by Longman (1960) who used an acceleration technique which is a variation of Euler's transformation; and (ii) by Sugihara (1987) who used Richardson's extrapolation, by considering the integral $\int_0^\infty e^{-ax^2} dx$ with $a = 2^{-n}$ for $n = 0, 1, \dots$. An alternative method was provided by Toda and Ono (1978) who used e^{-ax} instead of e^{-ax^2} and then computed the integral $I_0^\infty(wf)$ by applying a double exponential transformation of the form $x = \exp(y - e^{-y})$, followed by the trapezoidal rule. As discussed in §1.7.3, the Shanks accelerator technique was used by Alaylioglu, Evans and Hyslop (1973) to improve upon Longman's method. The method of Alaylioglu et al. involves a partition of the interval of integration according to the half-cycles of the integrand into subintervals $[t_n, t_{n+1}]$, $n = 0, 1, 2, \dots$. Thus, for 4.4.11, $t_n = n\pi/k$ for $w(x) = \cos kx$ or $\sin kx$, and $t_n = \sqrt{n\pi/k}$ for $w(x) = \cos kx^2$ or $\sin kx^2$. In both cases a low order p -point Gauss-Legendre quadrature formula is used over each

half-cycle $[t_n, t_{n+1}]$, which is

$$\int_{t_n}^{t_{n+1}} g(x) \, dx = \frac{t_{n+1} - t_n}{2} \sum_{i=1}^m w_i g\left(\frac{t_{n+1} - t_n}{2} + \frac{t_{n+1} - t_n}{2} x_i\right) + E_m, \tag{4.4.1}$$

where $g(x)$ represents a typical integrand, and m is taken at most 24. To minimize truncation and round-off errors, formula (4.4.1) is applied to each subinterval $[t_n, t_{n+1}]$, which yields the value $T_n = \int_{t_n}^{t_{n+1}} g(x) \, dx$, and the actual integrals required are given by $A = \sum_{i=1}^\infty T_i$. But Shanks accelerator technique is applied to the partial sums $A_n = \sum_{i=0}^n T_i$.

EXAMPLE 4.4.1. (Evans 1993) To compute

$$I_1(\alpha, k) = \int_0^\infty e^{-\alpha x} \sin kx \, dx = \frac{k}{\alpha^2 + k^2},$$

the sequence $\{A_n\}$ is given by

$$A_n = \frac{k}{\alpha^2 + k^2} \left[1 - (-1)^{n+1} e^{-(n+1)\alpha\pi/k} \right]. \tag{4.4.2}$$

If the transformation e_1 is applied to the sequence $\{A_n\}$, it converges geometrically to $B_{1n} = \frac{k}{\alpha^2 + k^2}$ for all n . However, by Longman’s method (Euler transformation), we obtain a sequence which exhibits an accelerated convergence for values of α less than the critical value $c_\alpha = k \ln 3/\pi$, but if $\alpha > c_\alpha$, the convergence becomes less rapid. Thus, Shanks technique gives faster convergence. ■

EXAMPLE 4.4.2. (Evans 1993) Consider $\int_0^\infty \frac{1}{x} e^{-x^2} \sin x \, dx = \tan^{-1} 2 \approx 1.107148718$. The Shanks transformation e_1 is applied iteratively to the sequence $\{A_n\}$ and we obtain the sequences $e_1\{A_n\}$, $e_1^2\{A_n\}, \dots$. Some of the initial elements of these sequences are given in Table 4.4.2. The half-cycle contributions T_n are computed over the subintervals $[n\pi, (n+1)\pi]$ using 16-point Gauss-Legendre formula (4.4.1), and the results are compared with the Euler’s transformation which when applied to T_n produces the sequence of partial sums S_n . ■

Table 4.4.2.

n	T_n	A_N	S_n	$e_1\{A_n\}$	$e_2\{A_n\}$
0	1.148148	1.148148	0.574074		
1	−0.045820	1.102328	0.849656	1.107254	
2	0.005519	1.107847	0.982409	1.107141	1.10749
3	−0.000809	1.107038	1.046562	1.107150	
4	0.000130	1.107163	0.077652		

EXAMPLE 4.4.3. (Evans 1993) Consider

$$\int_{\pi}^{\infty} x^{-2} \sin x \, dx = -\text{Ci}(\pi) \approx -0.0736679120464256.$$

The half-cycle computations over the subintervals $[(n+1)\pi, (n+2)\pi]$ are done by using a 16-point Gauss-Legendre formula (4.4.1). The results are presented in Table 4.4.3 (next page), where all entries must be multiplied by 10^{-2} . ■

EXAMPLE 4.4.4. (Evans 1993) Consider $\int_0^{\infty} x^2 \sin(100x^2) \, dx = \frac{1}{4000} \sqrt{\frac{\pi}{2}} \approx 3.13328534328875 \times 10^{-4}$. This integral converges in the mean only. The numerical values are obtained by using the integrating factor $e^{-\beta x^2}$ as $\beta \rightarrow 0$. The half-cycle contributions T_n with $t_n = \sqrt{n\pi/100}$ are obtained by 12 two-point Gauss-Legendre formula (4.4.1). The original sequence $\{A_n\}$ is found to be divergent. The results are given in Table 4.4.4 (next page), where it is found that the sequences $\{S_n\}$ and $e_1\{A_n\}$ converge slowly, but the sequences $e_1^2\{A_n\}$ and $e_1^3\{A_n\}$ converge rapidly. ■

4.4.2. Pantis' Method. Pantis (1975) extends Filon's method to infinite interval of integration by partitioning this interval into $[0, \alpha]$ and $[\alpha, \infty]$, and then applies Filon's method to the subinterval $[0, \alpha]$ while estimates the contribution from the interval $[\alpha, \infty]$ by using an asymptotic expression for large α . Thus, for example,

$$\int_0^{\infty} f(x) \sin(kx) \, dx = \left(\int_0^{\alpha} + \int_{\alpha}^{\infty} \right) f(x) \sin(kx) \, dx \equiv I_1(k) + I_2(k). \quad (4.4.3)$$

This method uses Filon's formula with the Gauss-Chebyshev rule for $I_1(k)$; for the integral $I_2(k)$ integration by parts gives

$$I_2(k) = \sum_{i=0}^M f^{(i)}(x) \frac{\cos^{(i)}(kx)}{k^{2i+1}} \Big|_{x=\alpha} + \int_{\alpha}^{\infty} f^{(M+1)}(x) \frac{\cos^{(M)}(kx)}{k^{2M+1}} \, dx. \quad (4.4.4)$$

This method is effective for very large k but fails if the derivatives of $f(x)$ cannot be easily found.

EXAMPLE 4.4.5. For $I_0^{\infty}(wf)$, where $w(x) = \sin(kx)$, the integral can be written in terms of the sinc transform as

$$S_n(k) = \int_0^{\infty} f(x) \sin(kx) \, dx = \sum_{n=0}^{\infty} u_n(x), \quad (4.4.5)$$

where

$$u_n(k) = (-1)^n \frac{1}{k} \int_0^{\pi} f\left(\frac{t+n\pi}{k}\right) \sin t \, dt. \quad (4.4.6)$$

Table 4.4.3.

n	T_n	A_N	S_n	$e_1\{A_n\}$	$e_1^2\{A_n\}$	$e_1^3\{A_n\}$
0	-9.6230(-2)	-9.6230(-2)	-4.8115(-2)			
1	3.3180(-2)	-6.3049(-2)	-6.3877(-2)	-7.3496(-2)		
2	-1.6737(-2)	-7.9786(-2)	-7.5529(-2)	-7.3744(-2)	-7.3677(-2)	
3	1.0078(-2)	-6.9708(-2)	-7.4305(-2)	-7.3633(-2)	-7.3667(-2)	-7.3669(-2)
4	-0.6730(-2)	-7.6439(-2)	-7.3901(-2)	-7.3689(-2)	-7.3670(-2)	
5	0.4812(-2)	-7.1626(-2)	-7.3614(-2)	-7.3657(-2)		
6	-0.3612(-2)	-7.5238(-2)	-7.3651(-2)			

Table 4.4.4.

n	T_n	A_N	S_n	$e_1\{A_n\}$	$e_1^2\{A_n\}$	$e_1^3\{A_n\}$	$e_1^4\{A_n\}$
0	1.2177(-3)	1.2177(-3)	6.0883(-4)				
1	-2.1650(-3)	-0.9474(-3)	3.7199(-4)	2.7356(-4)			
2	2.7998(-3)	1.8525(-3)	3.3292(-4)	3.3475(-4)	3.1236		
3	-3.3143(-3)	-1.4619(-3)	3.2090(-4)	2.9944(-4)	3.1366	3.1330	
4	3.7588(-3)	2.2970(-3)	3.1647(-4)	3.2324(-4)	3.1317	3.1332	3.1332
5	-4.1560(-3)	-1.8590(-3)	3.1468(-4)	3.0577(-4)	3.1340	3.1332	
6	4.5182(-3)	2.6593(-3)	3.1392(-4)	3.1931(-4)	3.1327		
7	-4.9535(-3)	-2.1943(-3)	3.1359(-4)	3.0842(-4)			
8	5.1671(-3)	2.9728(-3)	3.1344(-4)				

Then using Pantis' subdivision method, we write

$$I_0^\infty(wf) = \int_0^\alpha f(x) \sin(kx) dx + \frac{1}{k} f(\alpha) \cos(k\alpha) - \frac{1}{k^2} f'(\alpha) \sin(k\alpha) - \frac{1}{k^3} f''(\alpha) \cos(k\alpha) + \cdots, \quad (4.4.7)$$

where the asymptotic series (4.4.7) is valid for large k provided $f(\alpha)$ and its derivatives decrease rapidly. The choice of α is made by the relation $k\alpha = m\pi$, m an integer. Then this produces an asymptotic series of the form $(-1)^m \left[\frac{1}{k} f(\alpha) - \frac{1}{k^3} f''(\alpha) + \cdots \right]$, in which the odd derivatives are zero. However, if we want to compute $\int_0^\infty f(x) \sin(kx) dx$ for many values of k , the above choice of α would require new function evaluations for each k , and in that case α must be chosen independent of k (Pantis 1975). ■

4.4.3. Piessens' Method. To obtain a quadrature formula for

$$\int_a^b f(x) \frac{\sin(kx)}{\cos(kx)} dx,$$

consider the case of a function $f(x)$ which is very smooth on $[a, b]$ so that it can be approximated by a polynomial $Q_N(x)$ of high degree N . Then a quadrature formula has the form

$$\int_a^b f(x) \frac{\sin(kx)}{\cos(kx)} dx \approx \int_a^b Q_N(x) \frac{\sin(kx)}{\cos(kx)} dx. \quad (4.4.8)$$

If $a = -1$ and $b = 1$, Bakhvalov and Vasileva (1968) approximate $f(x)$ by a sum of Legendre polynomials $Q_N(x) = \sum_{j=0}^N c_j P_j(x)$, where the coefficients c_j are determined by interpolation in the zeros of $T_j(x)$. Then formula (4.4.8) becomes

$$S(k) \equiv \int_{-1}^1 f(x) \sin(kx) dx \approx \sum_{j=0}^{[(N-1)/2]} (-1)^j c_{2j+1} \sqrt{\frac{2\pi}{k}} J_{2j+3/2}(k), \quad (4.4.9a)$$

$$C(k) \equiv \int_{-1}^1 f(x) \cos(kx) dx \approx \sum_{j=0}^{[N/2]} (-1)^j c_{2j} \sqrt{\frac{2\pi}{k}} J_{2j+1/2}(k), \quad (4.4.9b)$$

where $J_n(x)$ is the Bessel function of the first kind and order n . A drawback with these formulas is that they are more complicated and develop serious round-off errors in computation.

Piessens and Poleunis (1971) modify the above formulas by using Chebyshev polynomials instead of Legendre polynomials. They use the Chebyshev expansion

$\sqrt{1-x^2} f(x) = \sum_{j=0}^N C_j T_j(x)$, and then approximate $f(x)$ by the truncated Chebyshev series

$$f(x) \approx \sum_{i=0}^N a_i T_i(x), \quad (4.4.10)$$

which gives a good approximation even with small N , where

$$\begin{aligned} a_i &\approx \frac{2}{N} \sum_{m=0}^N f\left(\cos \frac{\pi m}{N}\right) \cos \frac{im\pi}{N} \\ &= \frac{2}{N+1} \sum_{m=0}^N f(\cos x_m) \cos(ix_m), \quad x_m = \frac{(2m+1)\pi}{2(N+1)}. \end{aligned} \quad (4.4.11)$$

For an efficient computation of (4.4.10) one can use FFT (see §7.6). The values of N are determined in the same way as in the Clenshaw-Curtis quadrature method: If the approximation (4.4.10) is found to be insufficient for a certain value of N , simply double this value of N . This means that only N additional function evaluations are needed. The coefficients a_i are computed at nonequidistant nodes, which poses no problem if f is known analytically. Since $C_j = \frac{2}{\pi} \int_{-1}^1 f(x) T_j(x) dx$, we get

$$C_j \approx \frac{2}{\pi} \sum_{i=0}^N a_i \int_{-1}^1 T_i(x) T_j(x) dx,$$

or

$$\begin{cases} C_{2j} = \frac{2}{\pi} \sum_{i=0}^{[N/2]} a_{2i} \left[\frac{1}{(2i+2j)^2 - 1} + \frac{1}{(2i-2j)^2 - 1} \right], \\ C_{2j+1} = \frac{2}{\pi} \sum_{i=0}^{[(N-1)/2]} a_{2i+1} \left[\frac{1}{(2i+2j+2)^2 - 1} + \frac{1}{(2i-2j)^2 - 1} \right]. \end{cases}$$

Thus, formulas (4.4.9a,b) yield

$$S(k) \approx \sum_{j=0}^{[N/2]} C_j \int_{-1}^1 \frac{\sin(kx) T_j(x)}{\sqrt{1-x^2}} = \sum_{j=0}^{\infty} (-1)^j C_{2j+1} \pi J_{2j+1}(k), \quad (4.4.12a)$$

$$C(k) \approx \sum_{j=0}^{\infty} C_{2j} \pi J_{2j}(k), \quad (4.4.12b)$$

By Riemann-Lebesgue lemma, $C_j \rightarrow 0$ as $j \rightarrow \infty$, if $f(x)$ is absolutely integrable on $[-1, 1]$. Also, $J_n(k) \sim \frac{1}{\sqrt{2\pi n}} \left(\frac{ek}{2n}\right)^n$ as $n \rightarrow \infty$. Both series in (4.4.12) are

convergent and the terms decrease very rapidly for increasing j and $j > k/2$. Thus, these series can be truncated after M terms, where M is only slightly larger than $k/2$; this makes the truncation error negligible. The error E_S and E_C in $S(k)$ and $C(k)$ are

$$E_S \approx -2 \sin k \sum_{i=[(N+1)/2]}^{\infty} \frac{a_{2i+1}}{(2i+1)^2},$$

$$E_C \approx -\frac{\cos k}{2} \sum_{i=[N/2]+1}^{\infty} \frac{a_{2i}}{(i)^2},$$

respectively. Hence, as $N \rightarrow \infty$, the quadrature formulas (4.4.12a,b) converge faster than the Chebyshev series for $f(x)$. This method does not place any restriction on k .

EXAMPLE 4.4.6. To compute $\int_0^{2\pi} f_i(x) \sin(kx) dx$, $i = 1, 2, 3, 4$, where $f_1(x) = x \cos x$, $f_2(x) = x \cos(50x)$, $f_3(x) = \frac{x}{\sqrt{1-x^2/(4\pi^2)}}$, and $f_4(x) = \ln x$, Piesses and Poleunis (1971) compare the results from formula (4.4.12a) to those by Filon's formula and Gauss rule for radix 2 values of k (i.e., $k = 2^j$, $j = 0(1)8$) for $f_{1,2}(x)$, and for $k = 1, 2, 4, 10, 20, 30$ for $f_{3,4}(x)$ (see Davis and Rabinowitz 1967, where these integrands are used). They have found that the formulas (4.4.12) give superior results to Filon's rule. ■

EXAMPLE 4.4.7. (Piesses and Poleunis 1971) Consider $\int_{-1}^1 \frac{\sin(kx)}{x+3} dx$ with equidistant nodes at $x_j = -1 + 0.1j$, $j = 0(1)20$. The results are presented in Table 4.4.7 (next page). ■

4.4.4. Price's Method. Price (1960) considers integrals of the form

$$\int_0^{\pi} f(t) \sin t dt \approx \sum_{i=1}^N w_i f(t_i).$$

For $w(x) = \cos(kx)$, we can use the cosine transform and write

$$C(k) = \int_0^{\infty} f(x) \cos(kx) dx = \frac{1}{k} \int_0^{\pi/2} f\left(\frac{t}{k}\right) \cos t dt + \sum_{n=0}^{\infty} u_n(k), \quad (4.4.13)$$

where

$$u_n(k) = (-1)^{n+1} \frac{1}{k} \int_0^{\pi} f\left(\frac{t+n\pi+\pi/2}{k}\right) \sin t dt, \quad (4.4.14)$$

which is similar to (4.4.6) except that a separate computation of the integral over the interval $[0, \pi/2]$ is required in (4.4.13) which can be accomplished by using Gauss-Legendre or Gauss-Chebyshev quadrature rules, or even a Gauss-cos formula with

the weight function $\cos t$ on the interval $[-\pi/2, \pi/2$ and $[0, \pi/2]$. The coefficients for the Gauss-cos rule are given in [Tables A.16](#) and [A.17](#).

Table 4.4.7.

k	Exact	Filon’s Rule	(4.4.12a) $N = 4$
1	−0.071675	−0.076150	−0.071682
2	−0.103085	−0.109804	−0.103102
4	−0.025117	−0.027653	−0.025132
10	−0.019120	−0.021167	−0.019140
20	0.004379	0.005748	0.004386
30	0.001627	0.000935	0.001616

4.4.5. Use of Sinc Transform. Piessens and Haegemans (1973) and Boris and Oran (1975) use the sinc transform to obtain

$$S(k) = \int_0^\pi \sigma(t, k) \sin t \, dt, \tag{4.4.15}$$

where

$$\sigma(t, k) = \sum_{n=0}^\infty (-1)^n \frac{1}{k} f\left(\frac{t + n\pi}{k}\right).$$

This leads to the quadrature formula

$$S(k) \approx \frac{1}{k} \sum_{i=0} Nw_i \sum_{n=0}^\infty (-1)^n f\left(\frac{t_i + n\pi}{k}\right), \tag{4.4.16}$$

where the accelerator technique is used on the infinite sum prior to integration.

Thus, there are three basic methods: (i) the summation over the cycles (subintervals) is first carried out with or without accelerators and then is followed by integration. This is the ‘summation, then integration’ method which includes the work of Hurwitz and Zweifel (1956), Piessens and Haegemans (1973) and Boris and Oran (1975); (ii) ‘subdivision into half-cycles’ method, where integration is carried out over each half-cycle followed by computation of the resulting summation, mostly with the help of an accelerator; the work of Longman (1960), Alaylioglu, Evans and Hyslop (1973) and Squire (1973) discusses this method; and (iii) the ‘asymptotic expansion method’ together with a finite interval integrator as used in Pantis’ work (1975).

4.4.6. Test Integrals. The following integrals are evaluated.

$$I_1 = \int_0^\infty x \left(1 + x^2\right)^{-1} \sin x \, dx = \frac{\pi}{2e} \approx 0.5778636748954609$$
$$I_2 = \int_\pi^\infty x^{-2} \sin x \, dx = -\text{Ci}(\pi) \approx -0.0736679120464256$$

$$\begin{aligned}
I_3 &= \int_0^\infty x^{-1} e^{-x/2} \sin x \, dx = \tan^{-1}(2) \approx 1.10714871779409 \\
I_4 &= \int_0^\infty \operatorname{sech}(2x) \cos(4x) \, dx = \frac{\pi}{4} \operatorname{sech}(\pi) \approx 0.0677537378498546 \\
I_5 &= \int_0^\infty x^{-0.1} \sin x \, dx \\
&= \Gamma(0.9) \sin(0.45\pi) = \Gamma(0.9) \cos(0.05\pi) \approx 1.055472109508566 \\
I_6 &= \int_0^\infty x^2 \sin(100x^2) \, dx = \frac{1}{2} \int_0^\infty \sqrt{x} \sin(100x) \, dx \\
&\approx 3.133285343 \times 10^{-4} \\
I_7 &= \int_0^\infty \cos(1/x^2) \sin x^2 \, dx = \frac{\sqrt{\pi/2}}{4} (\cos 2 + \sin 2 + \cosh 2 - \sinh 2) \\
&\approx 0.1969225575949051 \\
I_8 &= \int_0^\infty x (1+x^2)^{-1} J_0(x) \, dx = K_0(1) \approx 0.4210244382407083 \\
I_9 &= \int_0^\infty x (1+x^2)^{-3} \sin(\omega x) \, dx \\
&= \begin{cases} \frac{3\pi}{64\sqrt{e}} \approx 0.0893190124092272 & \text{if } \omega = 0.5, \\ \frac{3\pi}{64e^3} \approx 0.1173080161711906 & \text{if } \omega = 3, \\ \frac{55\pi}{8e^{10}} \approx 0.00098056808998029 & \text{if } \omega = 10 \end{cases}
\end{aligned}$$

Note that the integral I_6 does not converge on $(0, \infty)$, and no exact solution is available. Mathematica gives this information: For the first part:

`I6 = NIntegrate [$x^2 * \sin[100x^2]$, { x , 0, ∞ }]`

the response is:

```

NIntegrate::"ploss": Numerical integration stopping due to loss
of precision. Achieved neither the requested
PrecisionGoal nor AccuracyGoal; suspect one of the following:
highly oscillatory integrand or the true value of the integral is
0. If your integrand is oscillatory try using the option Method
->Oscillatory in NIntegrate." and the result is  $-2.6603239458112698 \times 10^{115}$ 
which is not correct. However, the command
I6 = NIntegrate [ $x^2 * \sin[100x^2]$ , { $x$ , 0,  $\infty$ } Method -> Oscillatory]
yield the comment: SequenceLimit::"seqlim":
"The general form of the sequence could not be determined, and
the result may be incorrect." and the result 0.000313329, which in 16-point
precision (with SetPrecision[%, 16] command) is 0.0003133285343295913.

```

For the second part: the command `I6 = Integrate[Sqrt[x]*Sin[x]/2, {x, 0, ∞ }]` yields the comment: Integral of $\sqrt{x} \sin x$ does not converge on $(0, \infty)$.

4.5. Product Integration

We discuss some examples of the method of product integration, discussed in §3.7, which are relevant to infinite range integrals.

EXAMPLE 4.5.1. (Rabinowitz et al. 1987) Compute $\int_0^\infty e^{-x} f(x) dx$, where $f(x)$ is taken as $f_1(x) = e^x (1 + x^2)^{-1}$, $f_2(x) = \cos x$, $f_3(x) = \sin 5x$, and $f_4(x) = (1 + 0.02 x)^{-1}$, respectively, using positive interpolatory Gauss-Laguerre rules with k nodes, $k = 2, \dots, 20$. The results are given in Table 4.5.1.

EXAMPLE 4.5.2. Compute $\int_{-\infty}^\infty e^{-x^2} f(x) dx$, where $f(x)$ is taken as $f_5(x) = \sin^2 x$, $f_6(x) = (x^2 - 1) |x| \ln |x|$, $f_7(x) = x^2 e^x$, and $f_8(x) = \cos 4x^2$, respectively, using positive interpolatory Gauss-Hermite rule with k nodes, $k = 3(2)37$. The results are given in Table 4.5.2.

Table 4.5.1.

k	$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$
2	1.261	0.35	0.59	0.98064
3	1.487	0.39	0.57	0.9807562
4	1.488	0.39	0.56	0.9807562
5	1.449	0.508	-0.75	0.980755506
6	1.533	0.516	-0.12	0.9807554977
7	1.509	0.50095	0.73	0.9807554965
8	1.508	0.50104	0.68	0.9807554965
9	1.509	0.49913	0.17	0.9807554965
10	1.523	0.50020	0.38	0.9807554965
11	1.527	0.499976	0.307	0.9807554965
12	1.526	0.499977	0.303	0.9807554965
13	1.532	0.5000040	0.2955	0.9807554965
14	1.537	0.49999965	0.2962	0.9807554965
15	1.541	0.500000017	0.296155	0.9807554965
16	1.545	0.4999999996	0.29615682	0.9807554965
17	1.548	0.5000000000	0.29615678	0.9807554965
18	1.551	0.5000000000	0.29615678	0.9807554965
19	1.554	0.5000000000	0.29615678	0.9807554965
20	1.557	0.5000000000	0.29615678	0.9807554965
Exact	$\pi/2$	0.5	$5/26 \approx 0.19230769$	0.980755496569

Table 4.5.2.

k	$f_5(x)$	$f_6(x)$	$f_7(x)$	$f_8(x)$
3	0.586	0.013	1.47	0.1065
5	0.537	0.110	1.66	0.1156
7	0.553	0.116	1.713	0.1104
9	0.56014	0.568	1.706876	0.1158
11	0.560204	0.578	1.70690664	0.1160
13	0.56020235	0.566	1.706906845	0.1135
15	0.56020234	0.565	1.706906845	0.1134
17	0.5602022526	0.405	1.706906846	0.5859
19	0.5602022597	0.466	1.706906846	0.6059
21	0.5602022594	0.438	1.706906846	0.6949
23	0.5602022594	0.435	1.706906846	0.6818
25	0.5602022594	0.4331	1.706906846	0.6735
27	0.5602022594	0.43325	1.706906846	0.67414
29	0.5602022594	0.4332412	1.706906846	0.674110
31	0.5602022594	0.433141447	1.706906846	0.67411118
33	0.5602022594	0.4332414444	1.706906846	0.6741111694
35	0.5602022594	0.4332414444	1.706906846	0.6741111695
37	0.5602022594	0.4332414444	1.706906846	0.6741111695
Exact	0.56020226017	0.5	1.706906846	0.6880216946

5

Singular Integrals

Singular integrals are defined for unbounded integrands or over unbounded ranges of integration. These integrals do not exist as proper or improper Riemann integrals, but are defined as limits of certain proper integrals. The Gauss-Christoffel quadrature rule is discussed for singular integrals in general, and for those integrals that have singularities near and on the real axis. Product integration, endpoint and interior singularities and certain methods for acceleration of convergence are presented. Sidi's quadrature rules are studied, and tables are provided for the nodes and weights of the Gauss-Christoffel and Sidi's rules. Hypersingular integrals, specifically the Cauchy p.v. and the Hadamard finite-part integrals, are discussed.

5.1. Quadrature Rules

We consider $I_a^b(wf) = \int_a^b w(x) f(x) dx$. There are four cases of integrals where the integrand has a singularity. We will discuss these cases below where the singularity occurs at the endpoints of the interval of integration. The Gaussian quadrature method does not help in the cases when the singularity is of the form $1/\sqrt{1-x^2}$ on $[0, 1]$, or of the form $\sqrt{1-x^2}$ on $[0, 1]$, because of the derivative of the integrand that appears in the error term. However, as we have seen, the Gauss-Chebyshev quadrature works very well in the case of the singular term $1/\sqrt{1-x^2}$ on $[0, 1]$, since it becomes the weight function and is removed from the summation as well as the error term E_n (see §3.2.7).

CASE 1. $w(x) = \sqrt{1-x^2}$ on $[-1, 1]$. This is the Jacobi weight function with

$\alpha = \beta = 1/2$. The resulting orthogonal polynomials are the Chebyshev polynomials of the second kind $U_n(x)$ of degree n . The nodes, weights and error term for this quadrature are given by

$$x_i = \cos \frac{i\pi}{n+1}, \quad i = 1, \dots, n, \quad (5.1.1)$$

$$w_i = \frac{\pi}{n+1} \sin^2 \frac{i\pi}{n+1}, \quad (5.1.1a)$$

$$E_n = \frac{\pi}{2^{2n+1} (2n)!} f^{(2n)}(\xi), \quad -1 < \xi < 1. \quad (5.1.1b)$$

CASE 2. $w(x) = 1/\sqrt{x}$ on $[0, 1]$. In this case the singularity occurs at one endpoint. The orthogonal polynomials of degree n for this case are $p_n(x) = P_{2n}(\sqrt{x})$, where $P_{2n}(x)$ are the Legendre polynomials of degree $2n$. The nodes for the related quadrature are given by

$$x_i = \alpha_i^2, \quad i = 1, \dots, n, \quad (5.1.2)$$

where α_i are the positive zeros of $P_{2n}(x)$; the weights are given by

$$w_i = 2W_i, \quad (5.1.2a)$$

where W_i are the weights corresponding to α_i in the Gauss-Legendre quadrature of order $2n$, and the error term is given by

$$E_n = \frac{2^{4n+1} [(2n)!]^3}{(4n+1) [(4n)!]^2} f^{(2n)}(\xi), \quad 0 < \xi < 1. \quad (5.1.2b)$$

CASE 3. $w(x) = \sqrt{x}$ on $[0, 1]$. The singularity occurs in the derivative of the integrand at one endpoint. In this case the orthogonal polynomials of degree n are $p_n(x) = \frac{1}{\sqrt{x}} P_{2n+1}(\sqrt{x})$, where $P_{2n+1}(x)$ are the Legendre polynomials of degree $2n+1$. The nodes and the weights for the related quadrature are given by

$$x_i = \alpha_i^2, \quad i = 1, \dots, 2n+1, \quad (5.1.3)$$

$$w_i = 2W_i \alpha_i^2, \quad (5.1.3a)$$

where α_i are the positive zeros of $P_{2n+1}(x)$ and W_i are the weights corresponding to x_i in the Gauss-Legendre quadrature of order $2n+1$, and the error term is given by

$$E_n = \frac{2^{4n+3} [(2n+1)!]^4}{(4n+3) (2n)! [(4n+2)!]^2} f^{(2n)}(\xi), \quad 0 < \xi < 1. \quad (5.1.3b)$$

CASE 4. $w(x) = \sqrt{\frac{x}{1-x}}$ on $[0, 1]$. The weight function has a singularity at one endpoint and its derivative has a singularity at the other endpoint. In this case the

orthogonal polynomials of degree n are $p_n(x) = \frac{1}{\sqrt{x}} T_{2n+1}(\sqrt{x})$, where $T_{2n+1}(x)$ are the Chebyshev polynomials of the first kind of degree $2n+1$. The nodes, weights, and the error term for the related quadrature are given by

$$x_i = \cos^2 \frac{(2i-1)\pi}{4n+2}, \quad i = 1, \dots, 2n+1, \quad (5.1.4)$$

$$w_i = \frac{2\pi}{2n+1} x_i, \quad (5.1.4a)$$

$$E_n = \frac{\pi}{2^{4n+1} (2n)!} f^{(2n)}(\xi), \quad -1 < \xi < 1. \quad (5.1.4b)$$

EXAMPLE 5.1.1. (Ralston and Rabinowitz 1978, p. 112) Compute $I_0^1(f) = \int_0^1 \frac{1+x}{\sqrt{x}} dx$, for $n = 2$. From (5.1.2), and using the zeros of Legendre polynomials, we have

$$x_1 = (0.339981)^2 = 0.115587, \quad x_2 = (0.861136)^2 = 0.741555,$$

and from (5.1.2a) we get $w_1 = 1.304290$, $w_2 = 0.695710$. Thus, the approximate value of the integral is

$$I_0^1(f) \approx (1.304290)(1.115587) + (0.695710)(1.741555) = 2.666666.$$

This result compares very well with the exact value $8/3$. ■

5.1.1. Gauss-Christoffel Rules. (Gautschi 1968a) Let (a, b) denote a finite or infinite interval, and $w(x)$ be a nonnegative weight function defined on (a, b) such that $\int_a^b w(x) dx > 0$. We will discuss a sequence of quadrature rules $G_n(f)$

$$\int_a^b w(x) f(x) dx \approx \sum_{i=1}^n \lambda_i^{(n)} f(\xi_i^{(n)}), \quad n = 1, 2, \dots, \quad (5.1.5)$$

where $\xi_i^{(n)}$ are called the *Christoffel nodes*, and $\lambda_i^{(n)}$ the *Christoffel weights* associated with the weight function $w(x)$, and each rule is called a *Gauss-Christoffel quadrature formula*; the rule (5.1.5) is exact for $f \in \mathcal{P}_{2n-1}$. The moments μ_k with respect to $w(x)$, defined by $\mu_k = \int_a^b x^k w(x) dx$, $k = 0, 1, 2, \dots$, also exist. If $w(x)$ is not of a constant sign, the Gauss-Christoffel formulas still exist if certain Hankel determinants in the moments are nonzero (see [Stroud and Secrest 1966](#)). In this case some of the nodes $\xi_i^{(n)}$ may lie outside the interval (a, b) ; in particular, they may become complex.

The procedure to construct the formulas in (5.1.5) is as follows: Construct the system $\{q_i(x)\}$ of orthogonal polynomials associated with the weight function $w(x)$, and obtain $\xi_i^{(n)}$ as zeros of $q_n(x)$, and $\lambda_i^{(n)}$, in a number of ways, in terms of these

orthogonal polynomials. For example, Rutishauser (1963) uses the QD-algorithm, while Golub and Welsch (1969) use Francis' QR-transformation to compute $\xi_i^{(n)}$ as eigenvalues of a Jacobian matrix and $\lambda_i^{(n)}$ as the first components of the corresponding eigenvectors. These methods are computationally feasible for large n provided the orthogonal polynomials $q_n(x)$, or the associated Stieltjes continued fractions, are explicitly known. Otherwise, they exhibit a wide range of numerical instability, so much so that it becomes impossible to obtain any meaningful results unless multiple-precision computation is carried out.

The ill-conditioned nature of the problem is purely algebraic when one attempts to derive $\xi_i^{(n)}$ and $\lambda_i^{(n)}$ from the $2n$ moments of $w(x)$, i.e., solving the algebraic system of equations

$$\sum_{i=1}^n \lambda_i^{(n)} \left[\xi_i^{(n)} \right]^k = \mu_k, \quad k = 0, 1, \dots, 2n-1. \quad (5.1.6)$$

For a finite interval, say $(0, 1)$, the asymptotic relative condition number κ_n for this problem is given by

$$\kappa_n > \min \left(\mu_0, \frac{1}{\mu_0} \right) \max_{1 \leq i \leq n} \left\{ \left(1 + \xi_i^{(n)} \right) \prod_{k=1, k \neq i}^n \left[\frac{1 + \xi_k^{(n)}}{\xi_i^{(n)} - \xi_k^{(n)}} \right]^2 \right\}.$$

For $\mu_0 = 1$, the Table 5.1.1 presents the lower bound of κ_n , which is estimated by

$$\kappa_n > \min \left(\mu_0, \frac{1}{\mu_0} \right) \frac{(17 + 6\sqrt{8})^n}{64n^2} > \min \left(\mu_0, \frac{1}{\mu_0} \right) \frac{(33.97)^n}{64n^2}.$$

Table 5.1.1. Lower bound for Condition Number κ_n .

n	$(33.97)^n / 64n^2$
5	2.8(+4)
10	3.2(+11)
15	6.4(+18)
20	1.6(+26)

Thus, in the presence of round-off errors, the above mentioned rules that rely on moments will lose at least 11 decimal digits for $n = 10$, and 26 digits for $n = 20$. Hence, moments are not suitable for constructing the Gauss-Christoffel formulas. However, in §5.3 we will discuss Sidi's quadrature rules which are obtained after some rational approximations by applying a modification of Levin's nonlinear sequence transformation to the moment series of the weight function $w(x)$.

COMPUTATION OF CHRISTOFFEL WEIGHTS. The Christoffel weights $\lambda_i^{(n)}$ are computed by orthogonal polynomials of a discrete variable. Let $\{q_i^{(n)}\}_{i=1}^\infty$ denote

the associated orthonormal polynomial of degree i such that $\langle q_i, q_j \rangle = \delta_{ij}$. Let $\xi_n^{(n)}$ be the zeros of $q_n(x)$ in increasing order. Then $\xi_i^{(n)}$ are precisely the Christoffel nodes corresponding to the weight function $w(x)$. The Christoffel weights $\lambda_i^{(n)}$ can be determined, e.g., from

$$\lambda_i^{(n)} = \frac{1}{\sum_{k=0}^{n-1} [q_k(\xi_i^{(n)})]^2}. \quad (5.1.7)$$

We distinguish two cases: (i) the classical case, in which the orthogonal polynomials are known, and the problem is well-conditioned; and (ii) the nonclassical case, in which the orthogonal polynomials are *not* known and have to be generated. The first case uses an approximate discretization of orthogonality relation. In the second case, modified moments are used, and instead of the monomials $1, x, x^2, \dots$, one can orthogonalize any set of linearly independent polynomials. Thus, let $Q_N(\phi) = \sum_{k=1}^N w_k^{(N)} \phi(x_k^{(N)})$, $w_k^{(N)} > 0$, $N > n$, denote a sequence of auxiliary quadrature formulas

$$Q_N(\phi) \approx \int_a^b \phi(x) dx.$$

Let $(a, b) = (-1, 1)$. Then define a new inner product $\langle f, g \rangle_N = Q_N(fgw)$ by

$$\langle f, g \rangle_N = \sum_{k=1}^N W_k^{(N)} f(x_k^{(N)}) g(x_k^{(N)}), \quad (5.1.8)$$

where $W_k^{(N)} = w_k^{(N)} w(x_k^{(N)})$. Since $W_k^{(N)} > 0$ for $k = 1, 2, \dots, N$, the integrand (5.1.8) yields a set $\{q_{i,N}\}_{i=0}^{N-1}$ of orthogonal polynomials of a discrete variable such that $\langle q_{i,N}, q_{j,N} \rangle_N = \delta_{ij}$ for $i, j = 0, 1, \dots, N-1$. Now, define $\xi_{i,N}^{(n)}$ as the zeros of $q_{n,N}^{(n)}$, and let

$$\lambda_{i,N}^{(n)} = \frac{1}{\sum_{k=0}^{n-1} [q_{k,N}(\xi_{i,N}^{(n)})]^2}. \quad (5.1.9)$$

The quantities $\xi_{i,N}^{(n)}$ and $\lambda_{i,N}^{(n)}$, suitably ordered, are taken as approximations of $\xi_i^{(n)}$ and $\lambda_i^{(n)}$, respectively. The following conditions are imposed on the quadrature rules Q_n : (i) convergence should be reasonably rapid, even in the presence of singularities; (ii) the rule Q_n should be easy to generate for any, even large, values of N ; and (iii) the interval $[x_1^{(N)}, x_2^{(N)}, \dots, x_N^{(N)}]$ spanned by $x_1^{(N)}, x_2^{(N)}, \dots, x_N^{(N)}$ should contain the required Christoffel nodes $\xi_1 x_1^{(n)}, \xi_2^{(n)}, \dots, \xi_n^{(n)}$. Thus, N should not be excessively large. The process is feasible and avoids storage of a large number of high-order

quadrature formulas in the computer memory. Since the nodes $\xi_i^{(n)}$ show a tendency to crowd near the endpoints of ± 1 , we should choose the abscissae $x_k^{(N)}$ to have the same property. This rules out the use of most of the common quadrature rules, such as trapezoidal, midpoint, and Simpson's rules. The classical Gaussian quadrature rule is in conflict with the condition (ii). Only the N-C formula with the abscissae

$$x_k^{(N)} = \cos \theta_k^{(N)}, \quad \theta_k^{(N)} = \frac{2(k-1)\pi}{2N}, \quad (5.1.10)$$

which are the zeros of Chebyshev polynomials $T_n(x)$, as defined by Fejér formula, and the corresponding weights

$$w_k^{(N)} = \frac{2}{N} \left\{ 1 - 2 \sum_{m=1}^{[n/2]} \frac{\cos(2m\theta_k^{(N)})}{4m^2 - 1} \right\}, \quad (5.1.11)$$

comes close to satisfying all the above three conditions. Note that only one value of cosine, which is $\cos \frac{\pi}{2N}$, is needed in (5.1.10) and (5.1.11); the remaining values are then generated by well-known recurrence formulas. For best accuracy it is recommended that only the cosines in (5.1.11) be computed recursively, especially when N is very large.

Another suitable quadrature formula is the Gauss-Chebyshev formula defined by

$$\int_{-1}^1 \frac{\phi(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{N} \sum_{k=1}^N \phi(x_k^{(N)}),$$

which is written as

$$\int_{-1}^1 \phi(x) dx \approx \frac{\pi}{N} \sum_{k=1}^N (\sin \theta_k^{(N)}) \phi(x_k^{(N)}), \quad (5.1.12)$$

which is exact if $\phi(x) = p_{2N-1}(x) (1-x^2)^{-1/2}$, where $p_{2N-1}(x) \in \mathcal{P}_{2N-1}$. This formula is particularly suitable in cases where $w(x)$ has square-root singularities at the endpoint ± 1 . Note that the right side of (5.1.11) is the truncated Fourier series expansion of $\frac{\pi}{N} \sin \theta_k^{(N)}$, which is the weight factor in (5.1.12).

The process of constructing Christoffel numbers, based on the Fejér formula (5.1.10)-(5.1.11) is exact if $w(x)$ is a polynomial of degree m and $N > 2n + m$. Similarly, the process of constructing Christoffel numbers based on the Gauss-Chebyshev formula (5.1.12) is exact if $w(x) = (1-x^2)^{-1/2}$ and $N > n$.

ITERATIVE REFINEMENT OF CHRISTOFFEL NUMBERS. Let ξ_i^0, λ_i^0 be the approximations to the desired Christoffel numbers $\xi_i^{(n)}, \lambda_i^{(n)}$, which are sufficiently accurate when we solve the basic system of algebraic equations (5.1.6) by Newton's

method. Let $\{p_i\}_{i=0}^{2n-1}$ denote a system of $2n$ linearly independent polynomials, and define the ‘modified moments’ by

$$M_k = \int_a^b p_k(x) w(x) dx. \quad (5.1.13)$$

The basic system of equations (5.1.6) is then equivalent to

$$\sum_{i=0}^n \lambda_i^{(n)} p_k \left(\xi_i^{(n)} \right) = M - k, \quad k = 0, 1, \dots, 2n-1. \quad (5.1.14)$$

We wish to choose the polynomials p_k in such a way that the system (5.1.14), unlike (5.1.6), is well conditioned. For this purpose the ideal situation is to require that the Jacobian matrix $J(\lambda_1, \dots, \lambda_n; \xi_1, \dots, \xi_n)$ of (5.1.14) evaluated at the exact solution $\lambda_i = \lambda_i^{(n)}$, $\xi_i = \xi_i^{(n)}$ be orthogonal. But instead we consider orthogonality of $J(\lambda_1^0, \dots, \lambda_n^0; \xi_1^0, \dots, \xi_n^0)$. Since

$$J(\lambda_i; \xi_i) = \begin{bmatrix} p_0(\xi_1) & \cdots & p_0(\xi_n) & \lambda_1 p'_0(\xi_1) & \cdots & \lambda_n p'_0(\xi_n) \\ p_1(\xi_1) & \cdots & p_1(\xi_n) & \lambda_1 p'_1(\xi_1) & \cdots & \lambda_n p'_1(\xi_n) \\ \vdots & & \vdots & \vdots & & \vdots \\ p_{2n-1}(\xi_1) & \cdots & p_{2n-1}(\xi_n) & \lambda_1 p'_{2n-1}(\xi_1) & \cdots & \lambda_n p'_{2n-1}(\xi_n) \end{bmatrix},$$

we require that the rows in the above matrix be mutually orthogonal, which implies that the inner product $\{p_i, p_j\} = \delta_{ij}$ for $i, j = 0, 1, \dots, 2n-1$, where this inner product is defined by

$$\{f, g\} = \sum_{i=1}^n \left[f(\xi_i^0) g(\xi_i^0) + (\lambda_i^0)^2 f'(\xi_i^0) g'(\xi_i^0) \right].$$

Since the modified moments (5.1.13) are not known in advance, they must be generated along with the polynomials $p_i(x)$ with leading coefficient unity. These polynomials satisfy the recurrence relation

$$p_{k+1}(x) = (x - \alpha_k) p_k(x) - \beta_k p_{k-1}(x), \quad k \geq 1, \quad (5.1.15)$$

with $p_0(x) = 1$, $p_1(x) = x - \alpha_0$. If we put

$$h_k = \int_a^b w(x) \{p_k(x)\}^2 dx, \quad k = 0, 1, \dots, \quad (5.1.16)$$

then the coefficients of the recurrence relation (5.1.15) are given by

$$\beta_k = \frac{h_k}{h_{k-1}}, \quad k = 1, 2, \dots, \quad (5.1.17)$$

$$\alpha_k = \frac{1}{h_k} \int_a^b w(x) x \{p_k(x)\}^2 dx, \quad k = 0, 1, \dots. \quad (5.1.18)$$

If a is finite, then the recurrence relation (5.1.15) can be replaced by the system

$$\begin{aligned} p_{k+1}(x) &= (x - a) q_k(x) - \frac{\gamma_k}{h_k} p_k(x), \\ q_{k+1}(x) &= p_{k+1}(x) - \frac{h_{k+1}}{\gamma_k} q_k(x), \quad k = 0, 1, \dots, \end{aligned} \quad (5.1.19)$$

where

$$\gamma_k = \int_a^b w(x) (x - a) \{q_k(x)\}^2 dx, \quad (5.1.20)$$

and $\{q_k(x)\}_{k=0}^\infty$ is the set of polynomials with leading coefficient unity and orthogonal on (a, b) with respect to the weight function $w(x) (x - a)$. A similar result holds if b is finite. Since (5.1.15) and (5.1.19) are equivalent, we find that

$$\alpha_k = \frac{\gamma_k}{h_k} + \frac{h_k}{\gamma_{k-1}} + a. \quad (5.1.21)$$

The problem of generating the orthogonal polynomials $p_k(x)$ leads to the determination of the coefficients of the above recurrence relation, i.e., to compute the quadrature rules (5.1.16) and (5.1.18) (or (5.1.20)).

5.1.2. Logarithmic Weight Function. In order to construct the Gaussian rule for $\int_0^1 x^\alpha (-\ln x) dx$, $\alpha > -1$, we must find a computationally suitable expression for

$$I(g) = \int_0^1 x^\alpha (-\ln x) g(x) dx, \quad (5.1.22)$$

where $g(x)$ is a polynomial. Since

$$\begin{aligned} I(g) &= \int_0^1 dx x^\alpha g(x) dx \int_x^1 \frac{dt}{t} = \int_0^1 \frac{dt}{t} \int_0^t x^\alpha g(x) dx \\ &= \int_0^1 t^\alpha dt \int_0^1 u^\alpha g(ut) du, \end{aligned}$$

then, if $\{\lambda_i \xi_i\}_{i=1}^N$ is the N -point Gaussian rule for $\int_0^1 x^\alpha f(x) dx$, we get

$$I(g) = \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j g(\xi_i \xi_j) \quad (5.1.23)$$

for any polynomial $g(x)$ of degree $\leq 2N - 1$. Thus, for any $k < N$,

$$h_k = \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j \{p_k(\xi_i \xi_j)\}^2, \quad (5.1.24)$$

$$\alpha_k = \frac{1}{h_k} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j \xi_i \xi_j \{p_k(\xi_i \xi_j)\}^2, \quad (5.1.25)$$

Similarly from (5.1.5) we get

$$\gamma_k = \frac{1}{h_k} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j \xi_i \xi_j \{q_k(\xi_i \xi_j)\}^2. \quad (5.1.26)$$

Alternatively, another useful expression for h_k and γ_k is obtained as follows: Integration by parts gives

$$\int_0^1 (-\ln x) [x^{\alpha+1} g(x)]' dx = \int_0^1 x^\alpha g(x) dx.$$

Thus, for all $k < N$, we have

$$\begin{aligned} \sum_{i=1}^N \lambda_i \{p_k(\xi_i)\}^2 &= \int_0^1 (-\ln x) x^\alpha [(\alpha+1)p_k^2(x) + 2x p_k'(x) p_k(x)] dx \\ &= (2k + \alpha + 1) h_k, \end{aligned} \quad (5.1.27)$$

$$\sum_{i=1}^N \lambda_i \xi_i \{q_k(\xi_i)\}^2 = (2k + \alpha + 2) \gamma_k. \quad (5.1.28)$$

For $w(x) = \ln(1/x)$, $0 < x < 1$, the coefficients α_n and β_n of the recurrence relation (5.1.15) are given in Table A.18, and for $w(x) = E_1(x)$, $0 < x < \infty$, in Table A.19. The Christoffel nodes ξ_i and the weights λ_i for 10- and 20-point Gauss-Christoffel rule (5.1.5) for $w(x) = \ln(1/x)$, $0 < x < 1$, are given in Table A.20 and Table A.21, respectively; and those for 10- and 20-point rule in with $w(x) = E_1(x) = \int_0^\infty (e^{-xt}/t) dt$ are given in Table A.22 and Table A.23, respectively.

5.1.3. Singular Integrals. We will consider different methods to compute singular integrals of the form $\int_a^b f(x) g(x) dx$, where $g(x)$ is analytic and $f(x)$ is singular at one or both endpoints, or at an interior point. Let $F(x) = f(x) g(x)$. The interval of integration can always be transformed from $[a, b]$ to $[0, 1]$. For example, $f(x) = x^\alpha (\ln x)^\beta$ is singular at $x = 0$. If the singularity is at an interior point, then the interval $[a, b]$ is subdivided at the singularity and each subinterval is transformed to $[-1, 1]$ and the two integrals are treated separately. If $f(x)$ is singular at both endpoints, as e.g., $f(x) = x^{-\alpha} (1-x)^\beta$, $0 < \alpha, \beta < 1$, or $f(x) = \ln \ln x^{-1}$, then replace $F(x)$ by $\frac{1}{2} [F(x/2) + F(1-x/2)]$.

There are basically four approaches to compute singular integrals of the form mentioned above.

1. Ignore the singularity (Rabinowitz's method). If the singularity is taken out at an endpoint, then an open formula does not involve the evaluation of the integrand at its singular point. This approach involves a greater quadrature error as compared to that for a smooth integral, but it will eventually converge. Patterson's method and open Clenshaw-Curtis formulas (§3.3.1) are feasible for this case.

2. In some special cases a Gaussian formula with its requisite weight function removes the singularity. For example, for singularities of the following two types, we use the quadrature rules as follows: (i) for $f(x) = (1 - x^2)^{-1/2}$ on $[-1, 1]$ use the Gauss-Chebyshev quadrature; and (ii) for $f(x) = \ln x$ on $[-1, 1]$ use the Gauss-log quadrature. But a situation that arises with such Gaussian formulas concerns a nonstandard singularity, which does not have any specific formula. Sometimes the method known as ‘removing the singularity’ is used, as is done, e.g., for $I = \int_0^1 \ln x (1 + x^2)^{-1} dx$ which can be written as $I = \int_0^1 (\ln x (1 + x^2)^{-1} - \ln x) dx + \int_0^1 \ln x dx$ and simplifies to

$$I = - \int_0^1 x^2 (1 + x^2)^{-1} dx + \int_0^1 \ln x dx.$$

The first integral is nonsingular, but one must be careful with the computer code in avoiding the computation of $x^2 \ln x$ directly, since $x^2 \ln x \rightarrow 0$ as $x \rightarrow 0$. The second integral is obtained analytically.

3. The method known as ‘creeping up the singularity’ involves evaluating integrals whose range of integration approaches the singular point. This method generates a sequence of integrals and use of accelerators is needed to predict the required limit (see §1.6 on convergence accelerators).

4. This method uses transformations of the integrand by a suitable change of variables, which not only expunges the singularity but also has a zero endpoint derivative for the resulting integrand. The compound trapezoidal rule based on the Euler-Maclaurin summation formula (2.2.8) is a useful choice in this case.

5.1.4. Singularities near and on the Real Axis. Hunter (1992) has discussed a method for computing definite integrals $I_{-\infty}^{\infty}(f)$ where the integrand has singularities near the interval of integration on the real axis. A detailed study is found in Bialecki (1989). We consider the following cases.

1. f is analytic in some region containing the real axis except at the finite number of poles of arbitrary order which may be near but not on the real axis. We assume that the function f is real, i.e., $f(\bar{z}) = \overline{f(z)}$ for all complex $z = x + iy$. Although this assumption may not be necessary, the function f must satisfy the conditions: (i) f is integrable on the entire real axis; (ii) there is a real number $c > 0$ such that f is analytic over the region $D_c \subset \mathcal{C}$, defined by $D_c = \{z \in \mathcal{C} : |\Im\{z\}| \leq c\}$, except at a finite number of poles of arbitrary order within D_c ; and (iii) $f(R + iy) \rightarrow 0$ uniformly as $R \rightarrow \pm\infty$ for $|y| \leq c$. Then the method consists in the use of the following ‘shifted’ form of the trapezoidal rule:

$$T(\lambda, h) = h \sum_{k=-\infty}^{\infty} f((k + \lambda)h), \quad (5.1.29)$$

where $h > 0$ is a suitable interval and λ is a ‘shift’ parameter ($0 \leq \lambda \leq 1$). Then, if f has poles $z_1, z_2, \dots \in D_c$ such that none of them lies on the real axis, where z_m is

of order n_m , $m = 1, 2, \dots$, and if the principal part of the Laurent series of f about z_m is $\sum_{k=1}^{n_m} \rho_{mk} (z - z_k)^{-k}$, then

$$I_{-\infty}^{\infty}(f) = T^*(\lambda, h) + E(\lambda, h, c) \equiv T(\lambda, h) + R(\lambda, h, c) + E(\lambda, h, c), \quad (5.1.30)$$

where

$$R(\lambda, h, c) = 4\pi \Im \left\{ \sum_m^+ \frac{\rho_{m1}}{e^{2\pi i(z/h-\lambda)} - 1} \right\} + 2\pi \Re \left\{ \sum_m^+ \sum_{k=1}^{n_m} \rho_{mk} (\pi/h)^{k-1} G_k(\cot \pi(z_m/h - \lambda)) \right\}, \quad (5.1.31)$$

$$E(\lambda, h, c) = -2\Re \left\{ \int_{-\infty}^{\infty} \frac{f(x + ic)}{e^{-2\pi c/h - 2i\pi(x/h-\lambda)} - 1} dx \right\}, \quad (5.1.32)$$

and \sum_m^+ denotes summation over those poles $z_m \in D_c$ which lie above the real axis, and the functions G_k are defined by

$$G_k(\cot \alpha) = \frac{d^{k-1}}{d\alpha^{k-1}} \left\{ \frac{\cot \alpha}{(k-1)!} \right\}. \quad (5.1.33)$$

This method allows us to compute $I_{-\infty}^{\infty}(f)$ by applying the correction $R(\lambda, h, c)$ to the trapezoidal rule T^* , with the error term $E(\lambda, h, c)(\lambda, h)$. There are three aspects of the rule (5.1.30) that we will consider.

1. CHOICE OF c : The quantity c must be chosen large enough so that all poles of f near the real axis, which have significant effect on $T(\lambda, h)$ are contained in D_c . As c increases, the values of $R(\lambda, h, c)$ and $E(\lambda, h, c)$ change only when the horizontal edges of D_c pass through the poles. This indicates that the value of c must be precise as can be seen from the error bound (5.1.32)

$$|E(\lambda, h, c)| \leq \frac{2}{e^{2\pi c/h} - 1} \int_{-\infty}^{\infty} |f(x + ic)| dx, \quad (5.1.34)$$

which implies that the chosen value of c must be such that the right side of (5.1.34) remains minimal.

2. CHOICE OF λ : The role of the parameter λ is to control the effect of round-off errors. We must choose λ so that $R(\lambda, h, c)$ has the same sign as $T(\lambda, h)$ in the case of a pair of complex conjugate poles, say z_1 and $z_2 = \bar{z}_1$. But in the case when there are several pairs of conjugate complex poles it may become difficult to choose a λ that suits all. In particular, if g is an even function, the value $\lambda = 0$ or 0.5 should normally be used, so that the nodes $(k+1)h$ are symmetrically distributed about the real axis.

3. COMPUTATION OF $G_k(\cot \alpha)$: In view of the definition (5.1.33), we have $G_1(\cot \alpha) = \cot \alpha$, $G_2(\cot \alpha) = -\csc^2 \alpha$, and so on. But we will use the recurrence relations:

$$\begin{aligned} (2m-1)G_{2m}(\cot \alpha) &= -[G_m(\cot \alpha)]^2 \\ &\quad - 2 \sum_{j=1}^{m-1} G_j(\cot \alpha) \cdot G_{2k-j}(\cot \alpha), \quad m \geq 2, \\ 2mG_{2m+1}(\cot \alpha) &= -2 \sum_{j=1}^m G_j(\cot \alpha) \cdot G_{2k-j+1}(\cot \alpha), \quad m \geq 1. \end{aligned} \quad (5.1.35)$$

EXAMPLE 5.1.2. The integrand $f(z) = \frac{e^{-z^2}}{(z^2 + a^2)^3}$, $a > 0$ real, an even function and has conjugate poles of order 3 at $z_1 = ia$ and $z_2 = -ia$. The coefficients of the principal part of the Laurent series are

$$\rho_{11} = \frac{-ie^{a^2}(3 - 4a^2 + 4a^4)}{16a^5}, \quad \rho_{12} = \frac{-e^{a^2}(3 - 4a^2)}{16a^4}, \quad \rho_{13} = \frac{ie^{a^2}}{8a^3}.$$

The error from (5.1.34) is

$$\begin{aligned} |E(\lambda, h, c)| &\leq \frac{2}{e^{2\pi c/h} - 1} \int_{-\infty}^{\infty} \left| \frac{e^{-(x+ic)^2}}{[(x+ic)^2 + a^2]} \right| dx \\ &\leq \frac{2\sqrt{\pi} e^{c^2}}{e^{2\pi c/h} - 1} (c^2 - a^2)^3 \quad \text{provided } c > a. \end{aligned}$$

Since the maximum value of the expression on the right occurs when c is close to $\pi/2$, we get

$$|E(\lambda, h, c)| \leq \sqrt{\pi} \left(\frac{\pi^2}{h^2} - a^2 \right)^3 \operatorname{csch} \left(\frac{\pi^2}{h^2} \right) \left(\frac{\pi^2}{h^2} - a^2 \right)^3 \quad \text{provided } a < \pi/2.$$

Note that the integrand satisfies the criterion in (ii), which implies that we can take $\lambda = 0.5$. Then, for $a = 0.01$ and $h = 0.5$, we find that $|E(\lambda, h, c)| < 4.1235 \times 10^{-22}$. The following results are obtained:

For $\lambda = 0$: $T(0, 0.5) = 0.5 \times 10^{12}$; $R(0.0.5, c) = -0.48812942 \times 10^{12}$; thus, $T^*(0, 0.5, c) = 1.17805786 \times 10^{10}$.

For $\lambda = 0.5$: $T(0.5, 0.5) = 3832.681561$; $R(0.5, 0.5, c) = 1.1780376 \times 10^{10}$; thus, $T^*(0.5, 0.5, c) = 1.17805789 \times 10^{10}$. ■

5.1.5. Branch Singularities. The technique discussed above can be extended to deal with branch singularities. Consider a special case when $f(z) = (z^2 + a^2)^\alpha g(z)$, where $a > 0$ and α are real, $\alpha > -1$ and α not an integer, and g is

analytic inside a strip containing the real axis. As in (5.1.29)–(5.1.32), we integrate $\pi (z^2 + a^2)^\alpha g(z) \cot \pi(z/h - \lambda)$ around a suitable contour which is the rectangle with vertices at $\pm R \pm ic$. But if $c > a$, we must make slits in it to avoid the branch points at $\pm ia$. Eq (5.1.30) still holds, but now the correction term becomes

$$R(\lambda, h, c) = 2 \sin(\alpha\pi) \int_a^c (t^2 - a^2)^\alpha \left\{ \frac{g(it)}{e^{2\pi(t/h+i\lambda)} - 1} + \frac{g(-it)}{e^{2\pi(t/h-i\lambda)} - 1} \right\} dt, \quad (5.1.36)$$

which can be evaluated by setting $t = \frac{a + ce^{2u}}{1 + e^{2u}}$, so as to transform the interval $[a, c]$ into $(-\infty, \infty)$, and then use the trapezoidal rule.

EXAMPLE 5.1.3. Consider $\int_{-\infty}^{\infty} e^{-x^2} (x^2 + a^2)^{-1/2} dx$ which has the exact value $e^{a^2/2} K_0(a^2/2)$, where K_0 is the modified Bessel function of the second kind. For small a the branch points at $\pm ia$ are not easy to resolve. For example, for $a = 0.1$ we get $T(0.5, 0.5) = 4.43878372$; then, after using the trapezoidal rule with the interval $k = 0.25$, the correction (5.1.36) is $R(0.5, 0.5, 2\pi) = 1.0026444$; thus, $T^*(0.5, 0.5, 2\pi) = 5.44142820$; the exact value is 5.441428207737099, which is correct to 8 decimal places. ■

The method is deficient in (i) the restriction $\alpha > -1$; and (ii) the computation of $R(\lambda, h, c)$ which may involve a large number of function evaluations; there are 85 function evaluations for computing $R(\lambda, h, c)$ in Example 5.1.3. But if we do not use this method and use only the trapezoidal rule to compute $T(0.5, h)$, without the correction factor $R(0.5, h, c)$, we would require over 200 function evaluations with a value of $h < 0.02$.

5.1.6. Gautschi's Computation Codes. Gautschi (1994) has provided a collection of subroutines ORTHPOL and examples together with the underlying numerical methods which describe the procedures to generate orthogonal polynomials relative to arbitrary weight functions. The computer routines are useful in producing the coefficients of the three-term recurrence relation of the type (3.4.8) satisfied by the orthogonal polynomials. Once the coefficients are known, it is easy to generate additional data such as the zeros of orthogonal polynomials and Gaussian-type quadrature rules. Computer routines are provided for some of the well-known Gaussian rules, like Gauss-Radau and Gauss-Lobatto rules, discussed in §3.3.

5.1.7. Rational Gaussian Formulas. Gautschi (1999) has developed an algorithm GQRA that provides Gaussian quadratures that are exact for combinations of polynomials and rational functions, which are selected so as to simulate poles that may be presents in the integrands. The rational Gauss formula is of the form

$$\int_R f(t) d\lambda(t) = \sum_{k=1}^n \lambda_k f(x_k) + R_n(f), \quad (5.1.37)$$

Let $\omega_m(t) = \prod_{j=1}^M (1 + \zeta_j t)^{s_j}$ be a polynomial of exact degree m . Assume that the

measure $d\lambda/\omega_m$ admits an n -point Gaussian quadrature rule of the form

$$\int_R p(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{k=1}^n w_k^G p(\xi_k^G), \quad p \in \mathcal{P}_{2n-1}, \quad (5.1.38)$$

where the Christoffel nodes ξ_k are contained in the support of $d\lambda$. Define $\xi_k = \xi_k^G$, $\lambda_k = w_k^G \omega_m(\xi_k^G)$. Then we obtain the formula

$$\int_R g(t) d\lambda(t) = \sum_{k=1}^n \lambda_k g(\xi_k) + R_n(g), \quad (5.1.39)$$

where $R_n(g) = 0$ for all $g \in \mathcal{P}_{2n-1-m}$. Conversely, if (5.1.39) holds with $\xi_k \in \text{supp}(d\lambda)$, then so does (5.1.38) with ξ_k^G and w_k^G as defined above. The nodes for the rational Gauss formula are the Christoffel numbers (or nodes). Gautschi (1999) discusses the following examples.

EXAMPLE 5.1.4. $I_1(w) = \int_{-1}^1 \frac{(\pi t/w)}{\sin(\pi t/w)} dt$, $w > 1$. The integrand has simple real poles at the integral multiples of w . ■

EXAMPLE 5.1.5. $I_2(w) = \int_0^1 \frac{t^{-1/2} \Gamma(t+1)}{t+w} dt$, $w > 0$. Here $d\lambda(t) = t^{-1/2} dt$, and the integrand has poles at $-w$ and at negative natural numbers. ■

EXAMPLE 5.1.6. Generalized Fermi-Dirac integral

$$F_k(\eta, \theta) = \int_0^\infty \frac{t^k \sqrt{1 + \frac{\theta t}{2}}}{e^{-\eta+t} + 1} dt, \quad \eta \in \mathbb{R}, \theta \geq 0.$$

The values of k of physical interest are $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$. The following results are noteworthy: For $k = \frac{1}{2}$, $\eta = 1$ and $n = 5$, the integral has value 0.2905125 with a relative error of 0.39(−05). For this integral, also see Gautschi (1993), Lether (2000, 2001), and MacLeod (1998). ■

EXAMPLE 5.1.7. Generalized Bose-Einstein integral

$$G_k(\eta, \theta) = \int_0^\infty \frac{t^k \sqrt{1 + \frac{\theta t}{2}}}{e^{-\eta+t} - 1} dt, \quad \eta < 0, \theta \geq 0,$$

has poles that complex conjugate on the axis $\Im\{\xi\} = \eta$, at a distance of multiples of 2π from the real axis. Some results are as follows:

For $\eta = x = -0.001$, $\theta = 10^{-4}$, $k = \frac{1}{2}$:

$n = 6$, $m = 11$, the integral has value 0.2217149(+01) with a relative error of 0.2728(−06);

$n = 6, m = 5$, the integral has value 0.2217150(+01) with a relative error of 0.1653(-06);

$n = 6, m = 1$, the integral has value 0.2217150(+01) with a relative error of 0.1573(-06). ■

EXAMPLE 5.1.8. Radiation transfer integral

$$H_m(c) = 2 \int_0^1 P_m(x) [\sin(2\pi x)]^2 e^{-c/x} dx, \quad c > 0,$$

where $P_m(x)$ is the Legendre polynomial. It is found that

$$H_{50}(2) = \begin{cases} 0.29351229600590(-07) & \text{for } n = 26, \\ 0.29351229563622(-07) & \text{for } n = 27. \blacksquare \end{cases}$$

5.2. Product Integration

Rabinowitz and Smith (1992) study the product rules for $I_{-1}^1(kf)$ based on Gauss-Jacobi, Gauss-Radau and Gauss-Lobatto rules with the Jacobi weight function $w(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$, as applied to singular integrals, and determine sufficient conditions for convergence of these rules for both endpoint and interior singularities. Let $\{\bar{x}_{in}\}$ denote the nodes, and let $w(x) \in R[-1, 1]$. In the case of L_2 theory, there are no restrictions on w , but in the case of the L_p theory the weight function is restricted to the generalized smooth Jacobi (GSJ) weight function of the form

$$w(x) = \psi(x) \prod_{k=0}^N |x - t_k|^{\gamma_k}, \quad \gamma_k > -1, \quad N \geq 0 \quad (5.2.1)$$

$$-1 \leq t_0 < t_1 < \dots < t_{N+1} = 1,$$

where $\psi \in C[-1, 1]$, $\psi > 0$, and $\omega(\psi; t)$ denotes the modulus of continuity of the function ψ . The L_2 theory of product integration requires that both f and $K = k/w$ must belong to $L_{2,w}$. This theory is studied in detail for the Gauss-Jacobi nodes in Lubinsky and Sidi (1986), and extended to the Gauss-Radau and Gauss-Labatto nodes in Rabinowitz and Smith (1992). On the other hand, the L_p theory is based on the work of Nevai (1984) on weighted mean convergence of Lagrangian interpolation, where it is proved that product integration rules applied to bounded Riemann-integrable functions f converge under certain conditions on w and $k \in L_1[-1, 1]$.

For singular integrals, let the function f be unbounded at a finite set of nodes $Y = \{y_j, j = 1, \dots, l\} \subset [-1, 1]$, and we set $f(y_j) = 0$. In the L_2 case we can generally ignore the singularities, whereas in the L_p case the singularities can be generally avoided except in the case of the Jacobi weight function where they can be

ignored only in certain situations as noted in Rabinowitz (1987) and Vértesi (1989). Let

$$I_n(kf) = \sum_{i=1-r}^{n+s} w_{in} f(\bar{x}_{in}), \quad r, s \in \{0, 1\},$$

$$-1 = \bar{x}_{0n} < \bar{x}_{1n} < \dots < \bar{x}_{nn} < \bar{x}_{n+1,n} = 1, \quad (5.2.2)$$

where the weights $w_{in}(k)$ are chosen such that $I_n(kf) = I(kf)$, and the rule is exact if f is a polynomial of degree $< (n + r + s - 1)$. The nodes $\{\bar{x}_{in}\}$ are taken as the Gauss-Jacobi, Gauss-Radau and Gauss-Labatto points with respect to some $w \in \text{GSJ}$; i.e., they are the zeros of $q_{r+s+n}(x; w) = w_{rs}(x) p_n(x; \bar{w})$, where $\bar{w}(x) = w_{sr}(x) w(x)$, and for any $v \in \text{GSJ}$ we have $\{p_n(x; v) = k_n(v) x^n + \dots + k_n(v) > 0; n = 1, 2, \dots\}$ as a sequence of orthonormal polynomials with respect to the inner product $\langle f, g \rangle = I(vfg)$. If we denote the zeros of $p_n(x; v)$ by $x_{in}(v)$, $i = 1, \dots, n$, and the corresponding Gauss weights by $\mu_{in}(v)$ so that $I(vg) = \sum_{i=1}^n \mu_{in}(v) g(x_{in}(v)) + E_n g$, with $E_n(g) = 0$ if $g \in \mathcal{P}_{2n-1}$, we write the Gauss-Jacobi, Gauss-Radau and Gauss-Labatto rules with respect to w in a uniform manner as

$$I(wg) = \sum_{i=1-r}^{n+s} \bar{\mu}_{in} g(\bar{x}_{in}) + \bar{E}_n g, \quad (5.2.3)$$

where $\bar{\mu}_{in} = \mu_{in}(\bar{w})/w_{sr}(\bar{x}_{in}) > 0$, $i = 1, \dots, n$, and $\bar{E}_n g = 0$ if $g \in \mathcal{P}_{2n+r+s-1}$. If $g \in C^{2n+r+s}[-1, 1]$, then

$$\bar{E}_n g = (-1)^s \frac{g^{(2n+r+s)}(\xi)}{(2n+r+s)!} k_n(\bar{w})^{-2}, \quad -1 < \xi < 1. \quad (5.2.4)$$

In the Gauss-Jacobi case, $r + s = 0$, $\bar{w} = w$, $\bar{\mu}_{in} = \mu_{in}(w)$, and $\bar{x}_{in} = x_{in}(w)$; in the Gauss-Radau case, $r + s = 1$; and in the Gauss-Labatto case $r + s = 2$. The weights are $\bar{\mu}_{0n} > 0$ and $o(1)$ as $n \rightarrow \infty$ when $r = 1$, and $\bar{\mu}_{n+1,n} > 0$ and $o(1)$ as $n \rightarrow \infty$ when $s = 1$. The nodes $\bar{x}_{in} = \cos \theta_{in}$, $0 \leq \theta_{in} \leq \pi$, which implies that $\theta_{in} - \theta_{i+1,n} \sim n^{-1}$ uniformly for $0 \leq i \leq n$, $n = 1, 2, \dots$. Let $J = [-1, 1]$ and $T = \{t_j, j = 0, 1, \dots, N+1\}$. Then the weights $\bar{\mu}_{in}$ in any closed subinterval $J - T$ are such that $\bar{\mu}_{in} \sim n^{-1}$. The Lagrangian interpolation polynomials L_n for f at the zeros of $p_n(x; w)$ are defined by

$$L_n(x; w; f) = \sum_{i=1}^n l_{in}(x; w) f(x_{in}(v)),$$

$$l_{in}(x; w) = \frac{p_n(x; w)}{(x - x_{in}(w)) p'_n(x_{in}(w); w)}, \quad (5.2.5)$$

or

$$l_{in}(x; w) = \frac{k_{n-1}(w)}{k_n(w)} \mu_{in}(w) p_{n-1}(x_{in}(w); w) \frac{p_n(x; w)}{x - x_{in}(w)}.$$

The Lagrangian polynomials that interpolate f at the zeros of $q_{n+r+s}(x; w)$ are given by

$$\bar{L}_n(x; \bar{w}; f) = \sum_{i=1-r}^{n+s} \bar{l}_{in}(x; \bar{w}) f(x_{in}), \quad (5.2.6)$$

for certain polynomials $\bar{l}_{in}(w) \in \mathcal{P}_{n+r+s-1}$ such that $\bar{l}_{in}(\bar{x}_{in}; \bar{w}) = \delta_{ij}$. For $i = 1, \dots, n$, we have

$$\bar{l}_{in}(x; w) = \frac{w_{rs}(x)}{w_{sr}(\bar{x}_{in})} l_{in}(x; w). \quad (5.2.7)$$

Since $I_n(f; k) = I(k \bar{L}_n(\bar{w}; f))$, we have $w_{in}(k) = I(k \bar{l}_{in}(\bar{w}))$.

5.2.1. Endpoint Singularities. ($Y = \emptyset$) Rabinowitz and Smith (1992) have proved the following five theorem.

THEOREM 1. Let $f \in C[-1, 1]$, $w \in \text{GSJ}$, and $g = w_{cd}f$, where c, d are arbitrary but not necessarily such that $c, d > -1$. Let $v^* = w_{[c], [d]}$. Then

$$\int_{-1}^1 k(x) [g(x) - L_n(x; w; g)] dx \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (5.2.8)$$

if (i) $k \in L_1[-1, 1]$; (ii) $k v^* \in L \log^+ L[-1, 1]$; (iii) $k w^{-1/2} (1 - x^2)^{-1/4} \in L_1[-1, 1]$; and (iv) $v^* w^{1/2} (1 - x^2)^{1/4} \in L_1[-1, 1]$, where we have used the notation $h \in L \log^+ L[-1, 1]$ which means that $I(|h(\log |h|)|) < \infty$. This theorem is applicable only to the Gaussian rules for functions $g \in C[-1, 1]$. The strongest results occur when c and d are negative integers.

EXAMPLE 5.2.1. Consider $w(x) = (1 - x^2)^{-1/2}$, and $f \equiv 1$. The nodes $\{x_{in}(w)\}$ are the zeros of $T_n(x)$. If $g(x) = (1 - x^2)^{-m}$ so that $v^* = g$, the condition (ii) demands that $k(x) (1 - x^2)^{-m} \in L \log^+ L[-1, 1]$, i.e., k behave like $(1 - x^2)^{m-1+\varepsilon}$. Then conditions (i) and (iii) will be satisfied, but (iv) can hold only if $m = 0$. Thus, the above result is not applicable to the case of Chebyshev nodes, when there are endpoint singularities. ■

EXAMPLE 5.2.2. $w(x) = 1$, and $f \equiv 1$. The nodes $\{x_{in}(w)\}$ are the Gauss-Legendre points. If $g(x) = v^*(x) = (1 - x^2)^{-1}$, the condition (iv) is satisfied. If $k(x) (1 - x^2)^{-1} \in L \log^+ L[-1, 1]$, then all remaining conditions are satisfied; thus k must behave like $(1 - x^2)^\varepsilon$ near the endpoints so that $kg \in L_1[-1, 1]$. ■

EXAMPLE 5.2.3. $w(x) = (1 - x^2)^{1/2}$, and $f \equiv 1$. Then the nodes $\{x_{in}\}$ are the zeros of $U_n(x)$. If $g(x) = v^*(x) = (1 - x^2)^{-m}$, then the condition (iv) implies that m must be ≤ 1 . If we take $m = 1$, we are back to Example 5.2.2. ■

EXAMPLE 5.2.4. $w(x) = (1 - x^2)^{3/2}$, and $f \equiv 1$. The nodes $\{x_{in}(w)\}$ are the zeros of the Jacobi polynomial $P_n^{3/2, 3/2}(x)$. If $g(x) = v^*(x) = (1 - x^2)^{-m}$,

condition (iv) demands that $m \leq 2$. For $m = 2$, condition (ii) requires that $k(x)(1-x^2)^{-2} \in L \log^+ L[-1, 1]$, so that k behaves like $(1-x^2)^{1+\varepsilon}$ near the endpoints. With this choice of k the conditions (i) and (ii) are satisfied, so that the PIR converges for the strongly singular function $(1-x^2)^{-2}$. ■

In L_p theory, let $w \in \text{GSJ}$. and let $K = k/w \in L_{q,w}[-1, 1]$, where q is such that

$$\begin{aligned} \left| (c_0 + 1) \left(\frac{1}{q} - \frac{1}{2} \right) \right| &< \min \left\{ \frac{1}{4}, \frac{c_0 + 1}{2} \right\}, \\ \left| (c_{N+1} + 1) \left(\frac{1}{q} - \frac{1}{2} \right) \right| &< \min \left\{ \frac{1}{4}, \frac{c_{N+1} + 1}{2} \right\}, \\ \left| (c_k + 1) \left(\frac{1}{q} - \frac{1}{2} \right) \right| &< \min \left\{ \frac{1}{4}, \frac{c_k + 1}{2} \right\}, \quad k = 1, \dots, N. \end{aligned}$$

THEOREM 2. If $|f|^p$ is monotone integrable with respect to w and p , where $p^{-1} + q^{-1} = 1$, and if we set $f(\pm 1) = 0$, then $I_n(f; k) \rightarrow I(kf)$ as $n \rightarrow \infty$.

THEOREM 3. Let $w \in \text{GSJ}$ be such that $v = w/w_{sr} \in \text{GSJ}$, and assume that $K = k/w \in L_{q,v}$, where $p^{-1} + q^{-1} = 1$. If $|w_{sr}f|^p$ is monotone integrable with respect to v , then $I(k L_n(w; f)) \rightarrow I(kf)$ as $n \rightarrow \infty$.

EXAMPLE 5.2.5. If $w(x) = (1-x^2)^{-1/2}$, then q takes any value in $(1, \infty)$. For f to be as singular as possible, we must choose p close to 1. Then, if $f = (1-x^2)^\beta$, $\beta > -\frac{1}{2}$, so that $|f|^p$ is monotone integrable with respect to w , we determine the appropriate value of p , and the corresponding value of q would place the restriction on k that kf be in $L_1[-1, 1]$. Thus, if $k = (1-x^2)^\gamma$, then $\beta + \gamma > -1$, and all four conditions of Theorem 1 are satisfied; thus, the PIR based on the Chebyshev nodes converges for all f with $\beta > -1/2$, but Theorem 3 is not applicable since $w/w_{sr} \notin \text{GSJ}$. ■

EXAMPLE 5.2.6. If $w(x) = 1$, then $1 < q < 4$, which gives $p > 4/3$. If $f = (1-x^2)^\beta$, then β must be $> -3/4$. Using Theorem 2, the PIR based on Gauss-Legendre nodes converges only if f has a singularity weaker than $(1-x^2)^{-3/4}$. But since the condition on k is weaker than $(1-x^2)^{-3/4}$, we can allow a strong singularity on k ; for this we need $kf \in L_1[-1, 1]$ as in Example 5.2.5. Theorem 3 does not apply in this case. ■

EXAMPLE 5.2.7. If $w(x) = (1-x)^{1/2}$, then $1 < q < 3$, which gives $p > 3/2$ and $\beta > -1$. This case has good convergence. If we apply Theorem 3, we get a stronger result that permits us to take $\beta > -4/3$. ■

EXAMPLE 5.2.8. If $w(x) = (1-x)^{3/2}$, then $1 < q < 5/2$ so that $p > 2/3$ and $\beta > -3/2$. As in Example 5.2.6, this does not give as good a result as in Theorem 1. However, Theorem 3 weakens the condition on β , but it is not as good as $\beta \geq -2$ used in Examples 5.2.1–5.2.4. ■

5.2.2. Interior Singularities. Assuming that f has unbounded singularities

at the set $Y = \{y_j, j = 1, \dots, l\} \subset [-1, 1]$, we define $f(y_i) = 0$. Besides these singularities, there may be additional singularities at the endpoints ± 1 .

THEOREM 4. Let $w \in \text{GSJ}$, and $K/k/w \in L_{q,w}[-1, 1]$, where $p^{-1} + q^{-1} = 1$. If $|f|^p$ is monotone integrable with respect to w and Y for some $p > 1$, then

$$I_n(f; k) = \sum_{i \in \tau(n, f)} w_{in}(k) f(\bar{x}_{in}) \rightarrow I(kf) \quad \text{as } n \rightarrow \infty, \quad (5.2.9)$$

where $\tau(n, f)$ denotes a subset of $\{1, 2, \dots, n\}$ such that $i \in \tau(n, f)$ if either $Y \cap (\bar{x}_{i-1, n}, \bar{x}_{i+1, n}) = \emptyset$ or if for any j , $1 \leq j \leq l$, such that $y_j \in (\bar{x}_{i-1, n}, \bar{x}_{i+1, n})$, we have $\left| \int_{\bar{x}_{in}}^{y_j} w(x) dx \right| \geq \bar{\mu}_{jn}$. If $Y = \emptyset$, which means that there are only endpoint singularities, we have $\tau(n, f) = \{1, 2, \dots, n\}$.

THEOREM 5. Let $w \in \text{GSJ}$ be such that $v = w/w_{sr} \in \text{GSJ}$, and $K \in L_{q,v}[-1, 1]$, where $p^{-1} + q^{-1} = 1$. If $|w_{sr}f|^p$ is monotone integrable with respect to v , we have

$$I\left(k \hat{L}_n(w; f)\right) \rightarrow I(kf) \quad \text{as } n \rightarrow \infty, \quad (5.2.10)$$

where $\hat{L}_n(w; f) = \sum_{i \in \tau(n, f)} l_{in}(x; w) f(x_{in}(w))$.

For the sake of simplicity, we will assume that f has a single singularity at a point $\xi \in (-1, 1)$, $\xi \neq t_k$, $k = 1, \dots, N$. Let $M_d(\xi, k)$ denote the class of all functions g such that $g \in C(\xi, 1]$ and there exists an $F \geq 0$ on $[-1, 1]$ such that $F = 0$ on $[-1, \xi]$, F is continuous and nondecreasing on $(\xi, 1]$, $|f| \leq F$ on $[-1, 1]$, and $kF \in L_1[-1, 1]$. Then, if $w \in \text{GSJ}$, and $f \in M_d(\xi, k)$, $k(\xi) \neq 0$, and for some $p > 1$

$$\begin{cases} k \in L_p[-1, 1], \\ k w_{s-1/4, r-1/4} \bar{w}^{-1/2} \in L_p[-1, 1], \end{cases}$$

and k is either continuous or of bounded variation or satisfies a Lipschitz-Dini condition in $N_\delta(\xi) = [\xi, \xi + \delta]$, where δ is such that $N_\delta(\xi) \cap T = \emptyset$, we have $\tilde{I}_n(f, k) = I_n(f) - w_{\kappa n} f(x_{\kappa n}) \rightarrow I(kf)$ as $n \rightarrow \infty$, where κ is an index such that $x_{\kappa-1, n} \leq \xi < x_{\kappa n}$.

If w is the Jacobi weight function, then we can ignore the singularity in certain cases (see [Rabinowitz 1987](#), [Vértesi 1989](#)).

EXAMPLE 5.2.9. $w(x) = (1 - x^2)^\alpha$, $f(x) = (1 - x^2)^\beta$, and $k(x) = (1 - x^2)^\gamma$ with $\beta + \gamma > -1$. In L_2 theory, if $f \in L_{2,w}$ and $K \in L_{2,w}$, then, in view of Theorem 2, we must have $\beta > -(\alpha + 1)/2$ and $\gamma > (\alpha - 1)/2$. But in L_p theory, we must have $f \in L_{p,w}$ and $K \in L_{p,w}$, where we take $q \in (-1, \infty)$ when $\alpha \leq -1/2$, and $2 - \frac{2}{2\alpha + 3} < q < 2 + \frac{2}{2\alpha + 1}$ when $\alpha > -1/2$. Then β and γ must be such that $\beta > -\frac{2\alpha + 3}{4}$ and $\gamma > \frac{\alpha}{2} - \frac{1}{4}$. This permits us to deal with a singularity stronger

than $-1/4$. But in view of Theorem 3, α is restricted to $\alpha > 0$. Then in L_2 theory, β and γ must be such that $\beta > -(\alpha + 2)/2$ and $\gamma > \alpha/2$, whereas in L_p theory we must have $\beta > -\frac{\alpha}{2} - \frac{\alpha}{4\alpha + 4}$ and $\gamma > \frac{\alpha}{2} + \frac{\alpha}{4\alpha + 4}$, which is only a minor improvement. ■

5.3. Acceleration Methods

5.3.1. Endpoint Singularity. Consider the sequence $\{S_n\}$ defined by $S_n = \int_{x_n}^1 F(x) dx$. Then $S_n \rightarrow S$ as $n \rightarrow \infty$ only if $x_n \rightarrow 0$ as $n \rightarrow \infty$. The successive terms of this sequence are generated by $S_n = \sum_{i=1}^n T_i$, where

$$T_i = \int_{x_i}^{x_{i-1}} F(x) dx, \quad i \geq 1 \quad (5.3.1)$$

with $x_0 = 1$ and $x_n \rightarrow 0$ as $n \rightarrow \infty$. Amongst various choices of x_n , the most effective choice is $x_n = \theta^n$, $0 < \theta < 1$. The terms T_i in (5.3.1) are computed by the Patterson quadrature formulas of order 3, 7, 15, 31 ... (see Chapter 4). This method has high accuracy since the N -point Patterson formula is exact for a polynomial of degree $\leq (3N + 1)/2$. Also, the Patterson formulas are progressive in computation since they use the previous values as N increases.

EXAMPLE 5.3.1. Consider a simple singular integral: $\int_0^1 x^{-\alpha} dx$, $\alpha < 1$, for which $T_n = \gamma^{-1} \theta^{(n-1)\gamma} (1 - \theta^\gamma)$, $\gamma = 1 - \alpha$. Thus, the ratio $\frac{T_n}{T_{n-1}} = \theta^\gamma$, which is independent of n . Hence, the series for S_n has pure geometric convergence, and Aitkin's Δ^2 process (§1.6) will ensure convergence to the correct limit value from only the first three terms S_1, S_2, S_3 of the sequence $\{S_n\}$ for any value of θ , $0 < \theta < 1$. ■

In the general case, Shanks' diagonal transformation (Shanks 1955), as implemented by the ε -algorithm, is useful for computing integrals of the form $\int_0^1 x^{-\alpha} g(x) dx$. For such integrals, we have

$$\frac{T_n}{T_{n-1}} = \frac{\theta^\gamma g(\xi_n)}{g(\xi_{n-1})}, \quad x_n = \theta^n < \xi_n, \quad (5.3.2)$$

which does not exhibit pure geometric convergence. But the singularity at $x = 0$ is approached in the limit and we have $\lim_{n \rightarrow \infty} \frac{g(\xi_n)}{g(\xi_{n-1})} = 1$, which yields $\lim_{n \rightarrow \infty} \frac{T_n}{T_{n-1}} = \theta^\gamma$, and the ratio (5.3.2) exhibits almost pure geometric convergence for moderately large n or small θ .

5.3.2. Logarithmic Singularity. The integrals are of the form $\int_0^1 \ln x g(x) dx$. For $f(x) = \ln x$, we find that

$$T_n = f(\xi_n) \theta^{n-1} [n(1 - \theta) \ln \theta + \theta - 1 - \ln \theta].$$

Thus,

$$\frac{T_n}{T_{n-1}} = \frac{\theta(n-\tau)g(\xi_n)}{(n-1-\tau)g(\xi_{n-1})}, \quad \tau = \frac{\theta-1-\ln\theta}{(\theta-1)\ln\theta}.$$

Since $\lim_{\theta \rightarrow 1} \tau(\theta) = 1/2$ and $\lim_{\theta \rightarrow 0} \tau(\theta) = 1$, the function $\tau(\theta)$ increases monotonically from $1/2$ to 1 . The method again exhibits rapid geometric convergence for moderately large n or small θ . Hence, the ε -algorithm will provide rapid acceleration as in the case of endpoint singularity.

From these two cases it is obvious that the Patterson quadrature formulas together with the ε -algorithm are mostly effective for computing singular integrals. The parameter θ in $x_n = \theta^n$ plays an important role in the sense that large values of θ (close to 1) produce narrow intervals of integration, which require a minimum number of nodes for implementation of the quadrature formulas, and convergence in this case becomes very slow; on the other hand, small values of θ produce rapid convergence but computation process takes more time since $x_n \rightarrow 0$ (which is the singular point) slowly. From a practical point of view, one must refrain from approaching a distance of 10^{-p} of the singularity, where p is the machine precision of the computer used. Thus, the relation $\theta^n = 10^{-p}$ provides a ceiling on the value of n , which is $n = -p/(\log \theta)$. However, for safe computation, we should stay two orders of magnitude away from the singularity, which suggests the maximum value of n as $(2-p)/(\log \theta)$.

EXAMPLE 5.3.2. Evans, Hyslop and Morgan (1983) investigated the optimum choice of θ by computing many test integrals, some of which are:

$$\begin{aligned} I_1 &= \int_0^1 x^{-\alpha} dx = 10^6, \alpha = 1 - 10^{-6}; \\ I_2 &= \int_0^1 x^{0.95} e^x dx \approx 1.020457365236762; \\ I_3 &= \int_0^1 (\ln x)^2 (1+x^2)^{-1} dx \approx 1.937892292518698; \\ I_4 &= \int_0^1 \sqrt{x} e^{-x} (1+x)^{-1} dx \approx 0.2560043390094941. \end{aligned}$$

It is found that the classical Romberg halving choice of $\theta = 1/2$ was too large in many cases since it required a large number of terms (~ 20) for the ε -algorithm to achieve the desired accuracy. The smaller value $\theta = 0.1$ produced rapid convergence of the accelerated sequences $\{S_n\}$, but it also created computational problems due to the rapid approach to the singularity. Finally, the value $\theta = 0.2$ was assumed reasonable for all the above test integrals. Notice that the integral I_1 exhibits pure geometric convergence; the ratio $T_n/T_{n-1} \approx 1 + 10^{-6} \ln \theta \sim 1$, and therefore, an accurate value of T_i can be obtained by using 7- or 15-points Patterson quadrature formula. The integral I_2 , first studied by Cohen (1980), presented some computational problems when the Romberg halving technique was used; the integrals I_3 and I_4 have common singularities. According to Evans et al. (1983) the number of function evaluations (denoted by N_f) required to achieve a tolerance (relative error) of $E = 10^{-10}$ (denoted by $[*]$) for different choices of θ is shown in Table 5.3.2. ■

Table 5.3.2.

	$\theta = 0.1$ [Error]	$\theta = 0.2$ [Error]	$\theta = 0.5$ [Error]
I_1	45 [4.3(-6)]	21 [4.4(-6)]	21 [2.3(-6)]
I_2	32 [*]	27 [*]	40 [*]
I_3	102 [*]	111 [*]	91 [*]
I_4	105 [*]	127 [*]	184 [*]

EXAMPLE 5.3.3. The test integrals used by Chisholm, Genz and Rowlands (1972) are:

$$J_1 = \int_0^{2\pi} \ln x \sin x \, dx \approx -2.437653392946959;$$

$$J_2 = \int_0^1 x^{3/2} \, dx = 0.4;$$

$$J_3 = \int_0^1 x^{1/2} \ln x \, dx = -4/9;$$

$$J_4 = \int_0^1 x^{1/4} \cos x \, dx \approx 0.4451649230350326;$$

$$J_5 = \int_0^1 x^{-1/2} \, dx = 2;$$

$$J_6 = \int_0^1 (x^{1/2} + x^{1/3}) \, dx \approx 0.841116918071282;$$

$$J_7 = \int_0^1 \ln(1 - \cos x) \, dx \approx -2.721065445;$$

$$J_8 = \int_0^1 x^{-1/2} \ln x \, dx = -4;$$

$$J_9 = \int_0^\infty u e^{-u} (1 + u^2)^{-1} \, du = \int_0^1 t (1 + t^2)^{-1} \, dx \\ \approx 0.3433779615645852; \dagger$$

$$J_{10} = \int_0^\infty e^{-u} (1 + u)^{-1} \, du = \int_0^1 (1 + t)^{-1/2} \, dx \approx 0.7578721561656181; \dagger$$

$$J_{11} = \int_0^\infty e^{-u} u^{7/2} \, du = \int_0^1 t^{7/2} \, dx \approx 11.63172839718821; \dagger$$

$$J_{12} = \int_0^\infty e^{-u} (1 + u)^{-1} u^{-1/2} \, du = \int_0^1 t^{-1/2} (1 + t)^{-1/2} \, dx \\ \approx 1.343293414929015; \dagger$$

\dagger In these integrals $t = -\ln x$.

Chisholm et al. (1972) used the trapezoidal rule and a 2-point Gauss-Legendre rule with uniform partition into 2^p subintervals ($p = 0, 1, 2, \dots$), whereas Evans et al. (1983) used their own algorithm discussed above with a $2(p + 4)$ -point Gauss-Legendre sequence with arithmetic increase in the number of nodes, and a p -point Gauss-Legendre rule for the semi-infinite range with $\theta = 0.2$ and $E = 10^{-10}$. A comparison for the relative error E and the number of function evaluations N_f between these two methods is presented in Table 5.3.3. ■

EXAMPLE 5.3.4. Test function used by Harris and Evans (1977) and by Squire (1979) are:

$$H_1 = \int_0^1 \sqrt{x} \, dx = 1/3;$$

$$H_2 = \int_0^1 x^{-1/3} \, dx = 3/2;$$

$$H_3 = \int_0^1 x^{-2/3} dx = 3;$$

$$H_4 = \int_0^1 x^{7/2} dx = 2/9;$$

$$H_5 = \int_0^1 (\ln x)^2 dx = 2;$$

$$H_6 = \int_0^1 (\ln x)^4 dx = 24;$$

$$H_7 = \int_0^1 (1+x^2)^{-1} dx = \pi/4;$$

$$H_8 = \int_0^1 x^{-1/2} \ln x dx = -4;$$

$$H_9 = \int_0^1 (1 - \ln x)^{-1} (-\ln x)^{-1/2} dx \approx 1.34329342585706.$$

The results based on the three methods (Harris and Evans 1977, Squire 1979, and Evans et al. 1983 with $\theta = 0.2$) are compared in [Table 5.3.4](#). ■

EXAMPLE 5.3.5. Some test integrals with singularities at both endpoints are:

$$B_1 = \int_0^1 x^{-1/2} (1-x)^{-1/2} dx = \pi;$$

$$B_2 = \int_0^1 x^{-1/2} \ln \ln x^{-1} dx \approx 0.2318630313168279;$$

$$B_3 = \int_0^1 (1-x)^{-2} \ln \ln x^{-1} dx \approx -0.06281647980603772;$$

$$B_4 = \int_0^1 (-\ln x)^{-1} (-\ln x)^{-1} dx \approx 1.34329342585706;$$

$$B_5 = \int_0^1 \ln x \ln(1-x) dx \approx 0.3550659331472245;$$

$$B_6 = \int_0^1 (1-x)^{-1} \ln x dx \approx -1.644934066788805.$$

The results based on the three methods (Harris and Evans 1977, Squire 1979, and Evans et al. 1983 with $\theta = 0.2$) are compared in [Table 5.3.5](#). ■

Thus, we can easily conclude that the combined ε -Patterson procedure (Wynn 1956; Patterson 1968) seems to be very effective for a large number of singular integrals.

5.3.3. Levin's Transformations. (Sidi 1979b) Let $\{A_n\}_{n=1}^{\infty}$ be a sequence which converges to A as $n \rightarrow \infty$. Let $T_{k,n}$ denote the approximation to A , and γ_i , $i = 0, 1, 2, \dots, k-1$, be the solution to the $(k+1)$ linear equations

$$A_r = T_{k,n} + R_r \sum_{i=0}^{k-1} \frac{\gamma_i}{r^i}, \quad r = n, n+1, \dots, n+k, \quad R_r \neq 0. \quad (5.3.3)$$

A solution of these equations is given by

$$T_{k,n} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} A_{n+j} / R_{n+j}}{\sum_{j=0}^k (-1)^j \binom{k}{j} (n+j)^{k-1} / R_{n+j}} \quad (5.3.4)$$

$$= \frac{\Delta^k (n^{k-1} A_n / R_n)}{\Delta^k (n^{k-1} / R_n)}, \quad (5.3.5)$$

Table 5.3.3.

	Chisholm et al. (1972)		Evans et al. (1983)	
	N_f	$[E]$	N_f	$[E]$
J_1	60	$[1.1(-5)]$	57	$[1.0(-10)]$
J_2	62	$[1.0(-8)]$	29	$[1.0(-10)]$
J_3	65	$[6.2(-7)]$	59	$[1.0(-10)]$
J_4	65	$[1.0(-8)]$	51	$[1.0(-10)]$
J_5	62	$[9.1(-7)]$	45	$[1.0(-10)]$
J_6	62	$[1.9(-8)]$	49	$[6.7(-7)]$
J_7	65	$[1.0(-8)]$	65	$[8.2(-9)]$
J_8	65	$[2.5(-3)]$	59	$[4.0(-7)]$
J_9	65	$[5.1(-6)]$	59	$[3.3(-9)]$
J_{10}	55	$[2.7(-6)]$	47	$[1.2(-8)]$
J_{11}	55	$[5.2(-7)]$	59	$[1.9(-6)]$
J_{12}	65	$[2.3(-5)]$	55	$[3.2(-6)]$

Table 5.3.4.

	Harris and Evans (1977)	Squire (1979)	Evans et al. (1983)
	$E (N_f = 20)$	$E (N_f = 35)$	$E (N_f = 35)$
H_1	3.5(-6)	1.7(-6)	2.2(-8)
H_2	2.3(-4)	3.1(-6)	2.4(-7)
H_3	1.2(-2)	1.9(-3)	1.1(-6)
H_4	1.0(-10)	2.0(-5)	1.0(-10)
H_5	4.6(-4)	1.6(-6)	9.5(-4)
H_6	1.0(-2)	6.3(-5)	9.8(-2)
H_7	1.0(-10)	3.8(-6)	1.0(-10)
H_8	5.5(-3)	8.3(-4)	1.8(-6)
H_9	1.5(-6)	8.4(-5)	1.3(-5)

Table 5.3.5.

	Harris and Evans (1977)	Squire (1979)	Evans et al. (1983)
	$E (N_f = 20)$	$E (N_f = 35)$	$E (N_f = 35)$
B_1	7.5(-7)	7.1(-5)	6.4(-7)
B_2	6.7(-3)	1.5(-3)	6.2(-3)
B_3	1.3(-4)	1.1(-5)	2.8(-4)
B_4	1.5(-6)	8.4(-5)	1.3(-5)
B_5	3.3(-6)	4.0(-6)	1.7(-8)
B_6	3.6(-7)	2.0(-7)	1.7(-5)

where $\Delta^k \alpha_n = \sum_{j=0}^k (-1)^{k-j} \binom{k}{j} \alpha_{n+j}$. Let $a_1 = A_1$, and $a_r = \Delta A_{r-1}$, $r \geq 2$.

Some special cases are:

For the t -transformation: Take $R_r = a_r$;

For u -transformation: Take $R_r = r a_r$; and

For v -transformation: Take $R_r = a_r a_{r+1} / (a_{r+1} - a_r)$.

The t - and u -transformations deal with alternating and monotone series, respectively. It can be shown that

$$T_{k,n} - A = \frac{\Delta^k (n_{k-1} (A_n - A) / R_n)}{\Delta^k (n^{k-1} / R_n)}.$$

Let A_r be of the form

$$A_r = A + R_r f(r), \quad r = 1, 2, \dots, \quad (5.3.6)$$

where $f(x) \in C^\infty$ for all $x \geq n$, including $x = \infty$ and has a Poincaré-type asymptotic expansion $f(y) \sim \sum_{i=0}^{\infty} \frac{\beta_i}{x^i}$ as $x \rightarrow \infty$, $\beta_0 \neq 0$. Then for $w_k(x)$ defined by $w_k(x) = f(x) - \sum_{i=0}^{k-1} \frac{\beta_i}{x^i}$, Sidi (1979b) has proved that

$$T_{n,k} - A = \frac{\Delta^k [n_{k-1} w_k(n)]}{\Delta^k [n^{k-1} / R_n]}, \quad (5.3.7)$$

where $\Delta w_k(x) = w_k(x+1) - w_k(x)$.

The convergence properties of $T_{k,n}$ defined by (5.3.4) can be studied for two limiting processes: (i) k fixed, and $n \rightarrow \infty$; and (ii) n fixed, and $k \rightarrow \infty$. This study reveals the two noteworthy properties.

1. $T_{k,n}$ is a good approximation to A and converges to A very rapidly as $k \rightarrow \infty$ when A_r is of the form (5.3.6), where $f(x)$ has the asymptotic expansion $f(y) \sim \beta_0 + \frac{\beta_1}{x} + \frac{\beta_2}{x^2} + \dots$, as $x \rightarrow \infty$, $\beta_0 \neq 0$. The approximation $T_{k,n}$ is of no use in the case when A_r is not of the form (5.3.6).

2. Define $\bar{R}_r = R_r g(r)$, where $g(x)$ has the same properties as $f(x)$ and the limit $\lim_{x \rightarrow \infty} g(x) \neq 0$. Then (5.3.6) can be written as $A_r = A + \bar{R}_r \bar{f}(r)$, $r = 1, 2, \dots$, where $\bar{f}(r) = f(r)/g(r)$ and $\bar{f}(x)$ has the same properties as $f(x)$. Thus, the exact form of R_r in (5.3.6) is not important and R_r can be replaced by \bar{R}_r .

3. For $k \rightarrow \infty$ it is of no consequence if R_r in (5.3.4) is replaced by $r^s R_r$, where $s > 0$ is an integer which is not too large. But $s < 0$ destroys the accuracy of $T_{k,n}$.

5.3.4. Sidi's Rules. In Sidi (1980a) the integrals considered are of the form $I_0^1(wf)$, where the weight function $w(x)$ is of different forms defined in Table 5.3.6,

which contain the most important algebraic and logarithmic endpoint singularities.

Table 5.3.6.

$w(x)$	$\mu_m = \int_0^1 w(x) x^{m-1} dx$
1	$\frac{1}{m}$
x^β	$\frac{1}{m + \beta}, \quad \beta > -1$
$(1-x)^\alpha x^\beta$	$\frac{\alpha! (m + \beta - 1)!}{(m + \alpha + \beta)!}, \quad \alpha > -1, \beta > -1$
$(\log x)^\nu$	$\frac{\nu!}{m^{\nu+1}}, \quad \nu > -1$
$x^\beta (\log x)^\nu$	$\frac{\nu!}{(m + \beta)^{\nu+1}}, \quad \beta > -1, \nu > -1$
$(1-x)^\alpha x^\beta (\log x)^\nu$	No explicit expression for general α, β, ν , where $\beta > -1, \alpha + \nu > -1$

Let $f(z)$ be an analytic function in every finite subset of a simply connected (open) domain D of the complex plane which contains the real semi-infinite interval $[0, \infty)$. Let Γ denote a Jordan curve in D , which contains this semi-infinite interval in its interior. Then by Cauchy's theorem

$$f(z_0) = \frac{1}{2\pi i} \int_{\Gamma} \frac{f(z)}{z - z_0} dz, \quad (5.3.8)$$

where z_0 is an interior point of Γ . Define $A_0 = 0$, and $A_r = \sum_{m=1}^r \mu_m / z^m$. Then in the last case of $w(x)$ in Table 5.3.6, for every z not on the cut $[0, 1]$ we take $H(z) - A_{r-1}$ of the form $A_{r-1} = H(z) + R_r f(r)$, where $R_r = 1 / (r^{\alpha+\nu+1} z^r)$, and $f(x)$ is the same function as defined in (5.3.6). The n -point Sidi's rule S_k for the integral $I_0^1(wf)$ is given by the quadrature formulas

$$I_0^1(wf) \approx I_n(wf) = \sum_{i=1}^k w_{k,i} f(x_{k,i}), \quad k = 1, 2, \dots, \quad (5.3.9)$$

which are obtained after some rational approximations by applying a modification of Levin's nonlinear sequence transformation to the moment series of the weight function $w(x)$. In these formulas all the abscissae (nodes) $x_{k,i}$ lie in the interval $[0, 1]$ and their weights are all positive. In the case of endpoint singularities the nodes are the same and are independent of β . If $\alpha + \nu$ is a small nonnegative integer like 0, 1, 2, the same nodes can be taken in all cases of $w(x)$ listed in Table 5.3.6.

Since the nodes $x_{k,i}$, being the zeros of certain known polynomials, are known analytically, the corresponding weights $w_{k,i}$ are easily computed. The formulas (5.3.9)

possess very strong convergence properties and are as efficient as the corresponding Gaussian formulas.

For $w(x) = (1-x)^\alpha x^\beta (\log x)^\nu$, $\beta > -1$, and $\alpha + \nu \geq 0$ and very small like 0, 1, 2, the nodes $x_{k,i}$ are the roots of the polynomial equation $\sum_{j=0}^k \lambda_j z^j = 0$, where $\lambda_j = (-1)^j \binom{k}{j} (j+1)^k$, $j = 0, 1, \dots, k$. These nodes for $k = 2(1)12$ are presented in Table A.24.

Another Sidi's rule, denoted by \bar{S}_k , for $I_0^1(wf)$, which is of the form (5.3.9), has a different set of nodes $x_{k,i}$; they are the roots of the polynomial equation $\sum_{j=0}^k \lambda_j z^j = 0$, where $\lambda_j = (-1)^j \binom{k}{j} (j+1)^{k-1}$, $j = 0, 1, \dots, k$. Note that $z = 1$ is a node in \bar{S}_k . These nodes for $k = 2(1)12$ are presented in Table A.25.

For the weight functions $w(x) = x^\alpha e^{-x}$, $\alpha > -1$, and $w(x) = x^\alpha E_m(x)$, $\alpha > -1$, $\alpha + m > 0$, where $E_m(x)$ denotes the exponential integral $\int_1^\infty (e^{-xt}/t^m) dt$, let $A_0 = 0$, $A_r = \sum_{k=1}^r \mu_k/z^k$, $r = 1, 2, \dots$, and $R_r = \frac{(\alpha + r - 1)!}{z^r} r^{-1}$ for $r = 1, 2, \dots$. Then the modified T -transformation is given by

$$T_{k,n} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} (n+j)^{k-1} A_{n+j-1}/R_{n+j}}{\sum_{j=0}^k (-1)^j \binom{k}{j} (n+j)^{k-1}/R_{n+j}}, \quad (5.3.10)$$

Notice that the nodes $x_{k,i}$ are not symmetric with respect to $x = 0.5$ for $w(x) = 1$ or for any other weight function which is symmetric with respect to $x = 0.5$. Tables A.24 and A.25 show that many of the nodes $x_{k,i}$ cluster about $x = 0$ as k gets large. To obtain symmetric rules, consider the integral $I_{-1}^1(wf)$, where $w(x)$ is an even function, and define

$$\mu_m = \int_{-1}^1 w(x) x^{2(m-1)} dx, \quad m = 1, 2, \dots \quad (5.3.11)$$

Then

$$H(z) = \int_{-1}^1 \frac{w(x)}{z-x} dx = \sum_{m=1}^{\infty} \frac{\mu_m}{z^{2m-1}}. \quad (5.3.12)$$

Now, set $A_0 = 0$, $A_r = \sum_{m=1}^{\infty} \frac{\mu_m}{z^{2m-1}}$, $r = 1, 2, \dots$, and $R_n = \frac{c_r}{z^{2r-1}}$, $r = 1, 2, \dots$, in (5.3.4) and simplify the rational function for $T_{k,n}$ so obtained. Then $T_{k,n}$ will have simple poles if $n = 1$ or $n = 2$. For $n = 1$, the numerator of $T_{k,1}$ is an odd polynomial of degree $2k - 1$, and its denominator is an even polynomial of degree $2k$. Thus, $T_{k,1}$ gives a $2k$ -point quadrature rule. But for $n = 2$, the numerator of

$T_{k,2}$ is an even polynomial of degree $2k$, and its denominator is an odd polynomial of degree $2k + 1$. Thus, $T_{k,2}$ provides a $(2k + 1)$ -point quadrature rule. For these two rules, if ξ is a node, so is $-\xi$ and their corresponding weights are the same.

EXAMPLE 5.3.6. Consider $w(x) = 1$. Then $\mu_m = 2/(2m - 1)$, $m = 1, 2, \dots$. Choose $R_r = 1/(r z^{2r-1})$, $r = 1, 2, \dots$. Then the denominator of $T_{k,1}$ is

$$\sum_{j=0}^k \lambda_j z^{2j}, \quad \text{where } \lambda_j = (-1)^j \binom{k}{j} (j+1)^k, \quad j = 0, 1, \dots, k, \quad (5.3.13)$$

and the denominator of $T_{k,2}$ is

$$\sum_{j=0}^k \lambda_j z^{2j+1}, \quad \text{where } \lambda_j = (-1)^j \binom{k}{j} (j+2)^k, \quad j = 0, 1, \dots, k, \quad (5.3.14)$$

Thus, all the poles of $T_{k,1}$ and $T_{k,2}$ lie in $(-1, 1)$. If we replace $(j+1)^k$ in (5.3.13) by $(j+1)^{k-1}$ and $(j+2)^k$ in (5.3.14) by $(j+2)^{k-1}$, the endpoints ± 1 are also included in the nodes, thus giving (closed) Lobatto-type formulas. See [SidiNodes.nb](#) on the CD-R for computational details. ■

5.3.5. Infinite Range Integration. Sidi (1980b, 1982) has derived new interpolatory-type quadrature formulas for infinite range integrals which have algebraic or logarithmic endpoint singularities. Such integrals are of the form $I_0^\infty(wf)$, where $w(x) = x^\alpha e^{-x}$ or $w(x) = x^\alpha E_m(x)$, $\alpha > -1$, $\alpha + m > 0$. The modified T -transformation (5.3.4) becomes

$$T_{k,n} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} A_{n+j-1}/R_{n+j}}{\sum_{j=0}^k (-1)^j \binom{k}{j} (n+j)^{k-1}/R_{n+j}} \quad (5.3.15)$$

which, after cancelling a factor of z from the numerator and the denominator, yields

$$T_{k,n} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \frac{(n+j)^k}{(\alpha+n+j-1)!} A_{n+j-1}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \frac{(n+j)^k}{(\alpha+n+j-1)!} z^{n+j-1}}. \quad (5.3.16)$$

The n -point Sidi's rule \mathcal{S}_k for the integral $I_0^\infty(wf)$ is given by the quadrature formulas

$$I_0^\infty(wf) \approx J_n(f) = \sum_{k=1}^n w_{n,k} f(x_{n,k}), \quad (5.3.17)$$

where the nodes $x_{n,k}$ are distinct. Let

$$H(z) = \int_0^\infty \frac{w(x)}{z-x} dx, \quad H_k(z) = \sum_{i=1}^k \frac{w_{k,i}}{z-x_{k,i}}. \quad (5.3.18)$$

The function $H(z)$ is analytic in the z -plane cut along the positive real axis $[0, \infty)$ and has the divergent asymptotic expansion

$$H(z) \sim \sum_{n=1}^{\infty} \frac{\mu_n}{z^n} \quad \text{as } z \rightarrow \infty, z \notin [0, \infty), \quad (5.3.19)$$

where $\mu_n = \int_0^\infty w(x) x^{n-1} dx$ denote the moments of $w(x)$. If we require that the sequence of rational functions $H_k(z)$ tend to $H(z)$ uniformly and rapidly in any region of the complex plane that is at a finite distance from the positive real axis, then the error $E_k(f) = I_0^\infty(f) - I_k(f)$ will approach zero rapidly as $k \rightarrow \infty$. The success of Sidi's quadrature rule depends on assuming that $H(z)$ satisfies a relation of the form

$$H(z) = \sum_{i=1}^{n-1} \frac{\mu_i}{z^i} + R_n f(n), \quad (5.3.20)$$

where R_n depends on the moments, and $f(y) \in C^\infty[0, \infty)$ has an asymptotic expansion of the form $f(y) \sim \sum_{i=0}^{\infty} \frac{\beta_i}{y^i}$ as $y \rightarrow \infty$. Sidi has shown that (i) for $w(x) = x^\alpha e^{-x}$, $\alpha > -1$, the assumption (5.3.20) is satisfied for all $z \notin [0, \infty)$ with $M\mu_k = (\alpha + k - 1)!$ for $k = 1, 2, \dots$, $R_n = \frac{(\alpha + k - 1)!}{n z^n}$, and

$$f(y) \sim \sum_{k=0}^{\infty} \frac{-z e^{-z}}{y^k} \frac{\partial^k}{\partial \xi^k} \left[e^{(1-\alpha)\xi} \exp(z e^\xi) \right]_{\xi=0} \quad \text{as } y \rightarrow \infty;$$

and (ii) for $w(x) = x^\alpha E_m(x)$, $\alpha > -1$, $m + \alpha > 0$, with $\mu_k = \frac{(\alpha + k - 1)!}{m + \alpha + k - 1}$ for $k = 1, 2, \dots$, and R_n the same as in (i), and $f(y) \sim \sum_{k=0}^{\infty} \frac{-z \varepsilon_k(z)}{y^k}$ as $y \rightarrow \infty$, where

$$\varepsilon_k(z) = \frac{\partial^k}{\partial \xi^k} \left[e^{(1-\alpha)\xi} \exp(z e^\xi) \int_0^\xi e^{(1-m)u} \exp(-z e^u) du \right]_{\xi=0}.$$

The Sidi's k -point quadrature rule \mathcal{S}_k , defined by (5.3.17) for $I_0^\infty(wf)$, is derived using the modified T -transformation (5.3.16), which yields the following value of $H_n(z)$

valid for the weight functions $w(x) = x^\alpha e^{-x}$, $\alpha > -1$, and $w(x) = x^\alpha E_m(x)$, $\alpha > -1$, $m + \alpha > 0$:

$$H_k(z) = T_{k,1} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \frac{(j+1)^k}{(\alpha+j)!} z^j A_j}{\sum_{j=0}^k (-1)^j \binom{k}{j} \frac{(j+1)^k}{(\alpha+j)!} z^j} = \frac{N_{k,1}(z)}{D_{k,1}(z)}. \quad (5.3.21)$$

The nodes $x_{k,i}$ are the poles of $H_k(z)$; i.e., they are the zeros of the denominator $D_{k,1}(z)$ which are simple, and the weights $w_{k,i}$ are the residues of $H_k(z)$ at the corresponding $x_{k,i}$, given by

$$w_{k,i} = \left. \frac{N_{k,1}(z)}{D'_{k,1}(z)} \right|_{z=x_{k,i}}, \quad (5.3.22)$$

where $' \equiv d/dz$. The values of the nodes $x_{k,i}$ for $n = 2(1)12$ are given in Table A.24, and the corresponding weights $w_{n,k}$ for $w(x) = e^{-x}$ are given in Table A.25 and for $w(x) = E_1(x)$ in Table A.26. Note the slight difference between the results presented in the above tables and those given in Sidi (1980a, 1882a), which is due to the machine precision of different computers used in their evaluation. The nodes $x_{k,i}$ of Sidi's formulas $\int_0^\infty w(x) f(x) dx \approx \sum_{i=1}^k A_{k,i} f(x_i)$, where $w(x) = x^\alpha e^{-x}$ (Case 1), or $w(x) = x^\alpha E_p(x)$, $p > 1$ (Case 2), are given in Table A.27. The weights $A_{k,i}$ for these two cases are given separately, but the nodes remain the same in both cases.

5.4. Singular and Hypersingular Integrals

Let a function $f(x)$, $a \leq x \leq b$, be unbounded at some point $x_0 \in (a, b)$. Assume that f is Riemann integrable over the subintervals $[a, x_0 - \delta] \subset [a, x_0]$ and $(x_0 + \delta, b] \subset (x_0, b]$ for any $\delta > 0$. Then the *Cauchy's principal value (p.v.) integral* of f over $(a, b]$ is defined by

$$\int_a^b f(x) dx = \lim_{\delta \rightarrow 0^+} \left(\int_a^{x_0-\delta} f(x) dx + \int_{x_0+\delta}^b f(x) dx \right), \quad (5.4.1)$$

provided that this limit exists. The Cauchy's p.v. integral (5.4.1) is well defined whenever f is an improper Riemann-integrable on $[a, b]$. The point x_0 is called a weak singularity of f . For example, the function $f(x) = 1 + 1/x$ is not properly Riemann-integrable over $(0, 1]$, because

$$\lim_{\delta \rightarrow 0^+} \left(1 + \frac{1}{x} \right) dx = \lim_{\delta \rightarrow 0^+} [1 - \delta - \ln \delta] = +\infty.$$

Similarly, one can show that the improper integral of f over $[-1, 0)$ does not exist. But the Cauchy's p.v. integral of f over $[-1, 1]$ exists and is given by

$$\oint_{-1}^1 \left(1 + \frac{1}{x}\right) dx = \lim_{\delta \rightarrow 0^+} \left[\int_{-1}^{-\delta} \left(1 + \frac{1}{x}\right) dx + \int_{\delta}^1 \left(1 + \frac{1}{x}\right) dx \right] = 2. \blacksquare$$

In the case of an unbounded range of integration, let f be Riemann-integrable on all finite subintervals $[a, b] \subset R$. Then the *Cauchy's p.v. integral* of f over $(-\infty, \infty)$ is defined as

$$\oint_{-\infty}^{\infty} f(x) dx = \lim_{R \rightarrow \infty} \int_{-R}^R f(x) dx, \quad (5.4.2)$$

provided that this limit exists. As an example, consider $f(x) = x/(1+x^2)$, for which

$$\lim_{R \rightarrow \infty} \int_0^R \frac{x}{1+x^2} dx = \lim_{R \rightarrow \infty} \frac{1}{2} \ln(1+R^2) = +\infty.$$

Thus, this function is not improperly Riemann-integrable over $(-\infty, \infty)$, but its Cauchy's p.v. integral exists and has the value

$$\oint_{-\infty}^{\infty} \frac{x}{1+x^2} dx = \lim_{R \rightarrow \infty} \int_{-R}^R \frac{x}{1+x^2} dx = \lim_{R \rightarrow \infty} 0 = 0. \blacksquare$$

A common p.v. integral is the Hilbert transform $\oint_a^b \frac{f(t)}{t-x} dt$, where $-\infty \leq a < b \leq \infty$, and $a < x < b$. A sufficient condition for the Hilbert transform to exist over a finite interval $[a, b]$ is that $f(t)$ satisfy a *Lipschitz* or *Hölder* condition in $[a, b]$; i.e., there are constants $A > 0$ and $0 < \alpha \leq 1$ such that for any two points $t_1, t_2 \in [a, b]$ we have $|f(t_1) - f(t_2)| \leq A |t_1 - t_2|^\alpha$.

Another type of singular integrals is known as the *Hadamard finite-part integrals*, or *hypersingular integrals*; they are defined by

$$\begin{aligned} & \oint_a^b (x-a)^{\lambda-n} f(x) dx \\ &= \lim_{R \rightarrow a^+} \left[\int_R^b (x-a)^{\lambda-n} f(x) dx - g(R)(R-a)^{\lambda-n+1} \right], \end{aligned} \quad (5.4.3)$$

where $-1 < \lambda \leq 0$, $f \in C^n[a, b]$, $f(s) \neq 0$, and $g(R)$ is any function in $C^n[a, b]$ such that the limit exists and diverges for all positive integers n .

Consider a singular integral over the interval $[a, b]$ such that the integrand has a singularity of the type $\frac{1}{x-s}$ at an interior point s , $a < s < b$, and the regular part of the integrand is a function $\phi(x) \in C^0[a, b]$ that satisfies the Hölder condition

$$|\phi(x) - \phi(s)| \leq A |x-s|^\alpha,$$

where $0 < \alpha \leq 1$, and $|A| < \infty$. Then the Cauchy p.v. integral is defined by

$$\oint_a^b \frac{\phi(x)}{x-s} dx = \lim_{\varepsilon \rightarrow 0} \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{x-s} dx, \quad a < s < b, \quad (5.4.4)$$

where

$$\begin{aligned} \int_a^s \frac{\phi(x)}{x-s} dx &= \lim_{\varepsilon \rightarrow 0} \left\{ \int_a^{s-\varepsilon} \frac{\phi(x)}{x-s} dx - \phi(s) \ln \varepsilon \right\}, \\ \int_s^b \frac{\phi(x)}{x-s} dx &= \lim_{\varepsilon \rightarrow 0} \left\{ \int_{s+\varepsilon}^b \frac{\phi(x)}{x-s} dx + \phi(s) \ln \varepsilon \right\}, \end{aligned} \quad (5.4.5)$$

provided these limiting processes are taken together, since each of them does not exist independently. In fact, using the identity

$$\oint_a^b \frac{\phi(x)}{x-s} dx = \oint_a^b \frac{\phi(x) - \phi(s)}{x-s} dx + \phi(s) \oint_a^b \frac{dx}{x-s}$$

and (5.1.3), we find that

$$\oint_a^b \frac{\phi(x)}{x-s} dx = \oint_a^b \frac{\phi(x) - \phi(s)}{x-s} + \phi(s) \ln \frac{b-s}{s-a}, \quad (5.4.6)$$

since $\phi(x)$ satisfies the Hölder condition on $[a, b]$.

EXAMPLE 5.4.1. Let a Cauchy p.v. integral, denoted by $C_\nu(s)$, be defined by

$$C_\nu(s) = \oint_0^1 \frac{x^\nu}{x-s} dx, \quad 0 < s < 1, \quad \nu > -1.$$

Then the following results hold for rational ν :

$$\begin{aligned} \text{(i)} \quad C_{\nu+1}(s) &= s C_\nu(s) + \frac{1}{\nu+1}; \\ \text{(ii)} \quad C_\nu(s) &= -\pi s^\nu \cot \pi \nu - \sum_{n=0}^{\infty} \frac{s^{n-\nu}}{n-\nu} \quad -1 < \nu < 0, \nu \text{ not integer}; \\ \text{(iii)} \quad C_n(s) &= s^n \ln \left(\frac{1-s}{s} \right) + \sum_{k=1}^n \frac{s^{n-k}}{k} \quad \text{for integer } n. \end{aligned} \quad (5.4.7)$$

PROOF. (i) Take $x = x - s + s$; then

$$C_{\nu+1}(s) = \oint_0^1 \frac{x^{\nu+1}}{x-s} dx = \int_0^1 x^\nu dx + s \oint_0^1 \frac{x^\nu}{x-s} dx,$$

which proves the result.

(ii) For $-1 < \nu < 0$, set $x = su$; then

$$\begin{aligned}
 C_\nu(s) &= \oint_0^1 \frac{x^\nu}{x-s} dx = s^\nu \oint_0^1 \frac{x^\nu}{x-1} dx \\
 &= s^\nu \left[\int_0^\infty \frac{x^\nu}{x-1} dx - \int_{1/s}^\infty \frac{x^\nu}{x-1} dx \right] \\
 &= -\pi s^\nu \cot \pi \nu - s^\nu \int_0^s \frac{z^{-\nu-1}}{n-\nu} dz, \quad \text{where } x = 1/z, \\
 &= -\pi s^\nu \cot \pi \nu - \sum_{n=0}^\infty \frac{s^n}{n-\nu}, \quad -1 < \nu < 0, \nu \neq n,
 \end{aligned}$$

where we have used $\frac{1}{1-s} = \sum_{n=0}^\infty s^n$.

(iii) For $\nu = n$ (integer) we use recursion and get

$$\begin{aligned}
 C_0(s) &= \oint_0^1 \frac{1}{x-s} dx = \ln \left(\frac{1-s}{s} \right), \\
 C_1(s) &= \oint_0^1 \frac{x}{x-s} dx = 1-s \ln \left(\frac{1-s}{s} \right), \\
 C_2(s) &= \oint_0^1 \frac{x^2}{x-s} dx = \frac{1}{2} + s + s^2 \ln \left(\frac{1-s}{s} \right), \\
 C_3(s) &= \oint_0^1 \frac{x^3}{x-s} dx = \frac{1}{3} + \frac{s}{2} + s^2 + s^3 \ln \left(\frac{1-s}{s} \right),
 \end{aligned}$$

and so on. Thus, by induction we have

$$\begin{aligned}
 C_n(s) &= s^n \ln \left(\frac{1-s}{s} \right) + s^{n-1} + \frac{s^{n-2}}{2} + \cdots + \frac{1}{n} \\
 &= s^n \ln \left(\frac{1-s}{s} \right) + \sum_{k=1}^n \frac{s^{n-k}}{k}. \blacksquare
 \end{aligned}$$

EXAMPLE 5.4.2. If we denote the Cauchy p.v. integral by

$$I_{1,\nu} \equiv C_\nu(s) = \oint_0^1 \frac{x^\nu}{x-s} dx, \quad 0 < s < 1,$$

then by repeated differentiation we obtain the integral $I_{\alpha,\nu}$ for positive integer α as

$$I_{\alpha,\nu} = \oint_0^1 \frac{x^\nu}{(x-s)^\alpha} dx, \quad 0 < s < 1. \quad (5.4.8)$$

For proof, see [Bertram and Ruehr \(1992\)](#) and [Kythe and Puri \(2002\)](#). ■

5.4.1. P.V. of a Singular Integral on a Contour. Consider the singular integral

$$\int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta \quad \text{for } z, \zeta \in \Gamma,$$

on a contour Γ with endpoints a and b ($a = b$ if Γ is closed). Draw a circle of radius ρ with center at a point $z \in \Gamma$, and let z_1 and z_2 be the points of intersection of this circle with Γ . We take ρ small enough so that the circle has no other points of intersection with Γ . Let γ denote the part of the contour Γ cut out by this circle. Then the integral on the remaining contour $\Gamma - \gamma$ is $\int_{\Gamma - \gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta$, and the principal value of the singular integral (5.2.1) is given by $\lim_{\rho \rightarrow 0} \int_{\Gamma - \gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta$. Since

$$\int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta = \int_{\Gamma} \frac{\phi(\zeta) - \phi(z)}{\zeta - z} d\zeta + \phi(z) \int_{\Gamma} \frac{d\zeta}{\zeta - z},$$

we find in the same way that the singular integral (5.2.1) exists as a Cauchy p.v. integral for any function $\phi(\zeta)$ that satisfies the Hölder condition, and

$$\int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta = \int_{\Gamma} \frac{\phi(\zeta) - \phi(z)}{\zeta - z} d\zeta + \phi(z) \ln \frac{b - z}{z - a},$$

or

$$\int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta = \int_{\Gamma} \frac{\phi(\zeta) - \phi(z)}{\zeta - z} d\zeta + \phi(z) \left(\ln \frac{b - z}{z - a} + i\pi \right).$$

Moreover, if the contour Γ is closed, then we let $a = b$ and obtain

$$\int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta = \int_{\Gamma} \frac{\phi(\zeta) - \phi(z)}{\zeta - z} d\zeta + i\pi \phi(z).$$

Now consider the Cauchy-type integral

$$\Phi(z) = \frac{1}{2i\pi} \int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta, \quad (5.4.9)$$

where Γ is a closed or nonclosed contour and $\phi(\zeta)$ satisfies the Hölder condition on Γ . This integral has limit values $\Phi^+(z)$ and $\Phi^-(z)$ at any point $z \in \Gamma$ (z not equal to a or b) as $z \rightarrow \zeta$ from the left or from the right, respectively, along any path. These two limit values can be expressed in terms of the function $\phi(\zeta)$, which is known as the *density* of the integral, by the *Plemelj formulas*

$$\begin{aligned} \Phi^+(z) &= \frac{1}{2} \phi(z) + \frac{1}{2i\pi} \int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta, \\ \Phi^-(z) &= -\frac{1}{2} \phi(z) + \frac{1}{2i\pi} \int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta, \end{aligned} \quad (5.4.10)$$

such that

$$\begin{aligned}\Phi^+(z) + \Phi^-(z) &= \frac{1}{i\pi} \int_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta, \\ \Phi^+(z) - \Phi^-(z) &= \phi(z).\end{aligned}\tag{5.4.11}$$

If Γ is the real axis, then the Plemelj formulas become

$$\begin{aligned}\Phi^+(x) &= \frac{1}{2} \phi(x) + \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x} ds, \\ \Phi^-(x) &= -\frac{1}{2} \phi(x) + \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x} ds,\end{aligned}\tag{5.4.12}$$

and

$$\Phi^+(\infty) = \frac{1}{2} \phi(\infty), \quad \Phi^-(\infty) = -\frac{1}{2} \phi(\infty).\tag{5.4.13}$$

Hence, from (5.4.12) and (5.4.13) we have

$$\Phi^+(\infty) + \Phi^-(\infty) = 0, \quad \lim_{x \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x} ds = 0.\tag{5.4.14}$$

We use the first property in (5.4.14) to represent a piecewise analytic function in the upper and the lower half-plane by an integral over the real axis. Consider a Cauchy-type integral over the real axis:

$$\Phi(z) = \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(x)}{x - z} dx,\tag{5.4.15}$$

where z is complex and $\Phi(z)$ is a complex-valued function of a real variable x , which satisfies the Hölder condition on the real axis. If a function $\phi(x)$ is analytic on the upper half-plane D^+ , is continuous on the closed upper half-plane, and satisfies the Hölder condition on the real axis, then

$$\frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(x)}{x - z} dx = \begin{cases} \phi(z) - \frac{1}{2} \phi(\infty) & \text{for } \Im\{z\} > 0, \\ -\frac{1}{2} \phi(\infty) & \text{for } \Im\{z\} < 0; \end{cases}\tag{5.4.16}$$

also,

$$\frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(x) - \phi(\infty)}{x - z} dx = \begin{cases} \frac{1}{2} \phi(\infty) & \text{for } \Im\{z\} > 0, \\ -\phi(z) + \frac{1}{2} \phi(\infty) & \text{for } \Im\{z\} < 0, \end{cases}\tag{5.4.17}$$

provided $\phi(z)$ is analytic on the lower half-plane D^- , is continuous on the closed lower half-plane, and satisfies the Hölder condition on the real axis.

EXAMPLE 5.4.3. If $\Gamma = \{|z| = 1\}$, and $\phi(\zeta) = \frac{2}{\zeta(\zeta-2)} = \frac{1}{\zeta-2} - \frac{1}{\zeta}$, and $\phi(\infty) = 0$, then

$$\begin{aligned}\Phi(z) &= \frac{1}{2i\pi} \oint_{\Gamma} \frac{1}{\zeta-2} \frac{d\zeta}{\zeta-z} - \frac{1}{2i\pi} \oint_{\Gamma} \frac{1}{\zeta} \frac{d\zeta}{\zeta-z} \\ &= \begin{cases} \frac{1}{z-2} - \frac{1}{z} & \text{for } \Im\{z\} > 0, \\ \frac{1}{z} & \text{for } \Im\{z\} < 0, \end{cases}\end{aligned}$$

by (5.4.16) and (5.4.17). Hence,

$$\Phi^+(z) = \frac{1}{z-2} \quad \text{and} \quad \Phi^-(z) = \frac{1}{z}. \blacksquare$$

Another useful formula is the *Poincaré-Bertrand formula*:

$$\frac{1}{i\pi} \oint_{\Gamma} \frac{d\zeta}{\zeta-z} \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{\zeta-\zeta_1} d\zeta_1 = g(z, z) + \frac{1}{i\pi} \oint_{\Gamma} d\zeta_1 \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{(\zeta-z)(\zeta-\zeta_1)} d\zeta, \quad (5.4.18)$$

or, alternatively,

$$\oint_{\Gamma} \frac{d\zeta}{\zeta-z} \cdot \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{\zeta-\zeta_1} d\zeta_1 = \pi^2 g(z, z) + \oint_{\Gamma} d\zeta_1 \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{(\zeta-z)(\zeta-\zeta_1)} d\zeta, \quad (5.4.19)$$

where the function $g(\zeta, \zeta_1)$ satisfies the Hölder condition with respect to both variables. This formula is useful when changing the order of integration in singular integrals. Thus, the pair of iterated singular integrals

$$\begin{aligned}F(\zeta) &= \frac{1}{i\pi} \oint_{\Gamma} \frac{d\zeta}{\zeta-z} \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{\zeta-\zeta_1} d\zeta_1, \\ G(\zeta) &= \frac{1}{i\pi} \oint_{\Gamma} d\zeta_1 \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{g(\zeta, \zeta_1)}{(\zeta-z)(\zeta-\zeta_1)} d\zeta,\end{aligned}$$

are not equal, although they differ in the order of integration.

5.4.2. Application to Cauchy P.V. Integrals. For the sake of simplicity we assume that all poles z_1, z_2, \dots are simple and situated on the real axis. In such a case Eqs (5.1.30) and (5.1.32) still hold, but Eq (5.1.31) becomes

$$R(\lambda, h, c) = \pi \sum_m^+ \rho_{m1} \cot \pi \left(\frac{z_m}{h} - \lambda \right), \quad (5.4.20)$$

provided none of the values of $z_m/h - \lambda$ are integers. In the case of just one pole z_1 , we can choose λ such that $z_1/h - \lambda$ has a fractional part $\frac{1}{2}$, and thus, $R(\lambda, h, c) = 0$. In this way we try to avoid loss of accuracy which can occur if $T(\lambda, h)$ and $R(\lambda, h, c)$

are large and of opposite sign. But in the case of several poles we cannot choose λ and h easily, especially when f is an even function; then λ is chosen as 0 or 0.5.

EXAMPLE 5.4.4. Consider $f(z) = \frac{\operatorname{sech} z}{z - a}$, $a > 0$ real; this function has a simple pole at $z_1 = a$, with residue $\rho_{11} = \operatorname{sech} a$, which gives $R(\lambda, h, c) = \pi \operatorname{sech} a \cot \pi(a/h - \lambda)$. We take $\lambda = a/h - [a/h] \pm \frac{1}{2}$, where the sign \pm is chosen so that $0 \leq \lambda < 1$. Then $R(\lambda, h, c) = 0$, and $T^*(\lambda, h) = T(\lambda, h)$. For example, for $a = 0.1$, $h = 0.5$, we choose $\lambda = 0.7$; this gives $T^*(0.7, 0.5, c) = T(0.7, 0.5) = -0.2322322$. The error is given by $|E(\lambda, h, c)| \leq \frac{2\pi}{c} |\sec c| (e^{2\pi c/h} - 1)$, where $0 < c \leq \pi/2$, since the poles are at $\pm i\pi/2$. For $h = 0.5$ the maximum value of the error bound occurs at $c = 1.5$, which yields $|E(\lambda, h, c)| \leq 3.8564 \times 10^{-7}$. The accuracy can be improved by taking some of the poles on the imaginary axis at $z = (m - 0.5)i\pi$, with residue $\rho_m = \frac{(-1)^{m-1}\lambda}{a - (m - 0.5)i\pi}$. If we set $c = n\pi$ and let $n \rightarrow \infty$, then $E(\lambda, h, c) \rightarrow 0$, which implies that $I_{-\infty}^{\infty}(f) = T^*(\lambda, h) + S(\lambda, h)$, where

$$S(\lambda, h) = 4\pi \sum_{m=1}^{\infty} \Re \left\{ \frac{(-1)^{m-1}\lambda}{a - (m - 0.5)i\pi} \left(e^{(2m-1)\pi^2/h + 2\lambda i\pi} - 1 \right) \right\}. \quad (5.4.21)$$

The sum on the right converges very rapidly; for example, for $a = 0.1$, $h = 0.5$ and $\lambda = 0.7$ the first two terms in this sum are $-2.0691979 \times 10^{-8}$ and $4, 8873714 \times 10^{-26}$. ■

5.4.3. Hadamard's Finite-Part Integrals. Consider an improper integral on the interval $[a, b]$ such that (i) the integrand has a singularity of the type $\frac{1}{(x-s)^2}$ at an interior point s , $a < s < b$, and (ii) the regular part of the integrand is a function $\phi(x)$, $a \leq x \leq b$, which satisfies a Hölder continuous first-derivative condition

$$|\phi(x) - \phi(s) - (x-s)\phi'(s)| \leq A|x-s|^{\alpha+1},$$

where $0 < \alpha \leq 1$ and $|A| < \infty$, as before. Then a Hadamard's (finite-part) integral is defined by

$$\oint_a^b \frac{\phi(x)}{(x-s)^2} dx = \lim_{\varepsilon \rightarrow 0} \left\{ \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{(x-s)^2} dx - \frac{2\phi(s)}{\varepsilon} \right\}, \quad (5.4.22)$$

where the neighborhood ε is symmetric about the singular point s . This integral can also be evaluated on both sides of the singular point as first-order one-sided integrals

$$\begin{aligned} \int_a^s \frac{\phi(x)}{(x-s)^2} dx &= \lim_{\varepsilon \rightarrow 0} \left\{ \int_a^{s-\varepsilon} \frac{\phi(x)}{(x-s)^2} dx - \frac{\phi(s)}{\varepsilon} - \phi'(s) \ln s \right\}, \\ \int_s^b \frac{\phi(x)}{(x-s)^2} dx &= \lim_{\varepsilon \rightarrow 0} \left\{ \int_{s+\varepsilon}^b \frac{\phi(x)}{x-s} dx - \frac{\phi(s)}{\varepsilon} + \phi'(s) \ln s \right\}, \end{aligned}$$

both of which must be taken together.

Differentiation of the Cauchy p.v. integrals with respect to s is carried out by using the Leibniz rule (1.1.5), which yields

$$\begin{aligned} \frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s} dx &= \lim_{\varepsilon \rightarrow 0} \frac{d}{ds} \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{x-s} dx \\ &= \lim_{\varepsilon \rightarrow 0} \left\{ \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{(x-s)^2} dx - \frac{\phi(s-\varepsilon) + \phi(s+\varepsilon)}{\varepsilon} \right\}. \end{aligned} \quad (5.4.23)$$

Since ϕ is continuous on $a \leq x \leq b$, we have $\phi(s-\varepsilon) = \phi(s+\varepsilon) = \phi(s)$ as $\varepsilon \rightarrow 0$. Then formula (5.4.23) becomes

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s} dx = \lim_{\varepsilon \rightarrow 0} \left\{ \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{x-s} dx - \frac{2\phi(s)}{\varepsilon} \right\}, \quad (5.4.24)$$

which is the same as (5.4.22). Hence, we obtain the formula

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s} dx = \int_a^b \frac{\phi(x)}{(x-s)^2} dx, \quad (5.4.25)$$

which is very useful in evaluating Hadamard's finite-part integrals.

5.4.4. Two-Sided Finite-Part Integrals. If we take $\phi(x) = \phi(x) - \phi(s) + \phi(s)$ in the Cauchy p.v. integral (D.2.1), then

$$\int_a^b \frac{\phi(x)}{x-s} dx = \int_a^b \frac{\phi(x) - \phi(s)}{x-s} dx + \phi(s) \int_a^b \frac{dx}{x-s}, \quad (5.4.26)$$

where

$$\int_a^b \frac{dx}{x-s} = [\ln |x-s|]_a^b = \ln \left| \frac{b-s}{s-a} \right|. \quad (5.4.27)$$

If $\phi \in C^1[a, b]$, the continuity requirement on $\phi'(x)$ is a necessary condition for a Taylor's series expansion of the function $\phi(x)$. But if $\phi(x) \notin C^1$, i.e., it does not have a high degree of continuity so as not to allow a Taylor's series expansion, a sufficient condition for the existence of finite-part integral is that $\phi(x)$ satisfy a Hölder or Lipschitz condition, i.e., $|\phi(x) - \phi(s)| \leq A|x-s|^\alpha$, $0 < \alpha \leq 1$, $|A| < \infty$. This condition also guarantees that the first integral on the right side of (5.4.26) is, at most, weakly singular. Now, integrating (5.4.4) by parts we get

$$\int_a^b \frac{\phi(x)}{x-s} dx = \phi(b) \ln |b-s| - \phi(a) \ln |a-s| - \int_a^b \phi'(x) \ln |x-s| dx, \quad (5.4.28)$$

where $\phi(x) \in C^1[a, b]$. Then differentiation of (5.4.28) with respect to s yields

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s} dx = \frac{\phi(a)}{a-s} - \frac{\phi(b)}{b-s} + \int_a^b \frac{\phi'(x)}{x-s} dx, \quad (5.4.29)$$

where $\phi'(x)$ satisfies the Hölder condition $|\phi'(x_1) - \phi'(x_2)| \leq A|x_1 - x_2|^\alpha$.

Similarly, the finite-part integral of $\phi(x) \in C^2[a, b]$ is defined by

$$\begin{aligned} \oint_a^b \frac{\phi(x)}{(x-s)^2} dx &= \int_a^b \frac{\phi(x) - \phi(s) - (x-s)\phi'(s)}{(x-s)^2} dx \\ &+ \phi(s) \oint_a^b \frac{dx}{(x-s)^2} + \phi'(s) \int_a^b \frac{dx}{x-s}, \end{aligned} \quad (5.4.30)$$

where on the right side the last integral is evaluated in (5.4.27), while the second integral is given by

$$\oint_a^b \frac{dx}{(x-s)^2} = \left[-\frac{1}{x-s} \right]_a^b = \frac{1}{a-s} - \frac{1}{b-s}.$$

In the case when $\phi(x) \notin C^2$, i.e., it does not have a high degree of continuity to allow a Taylor's series expansion, a sufficient condition for the existence of the finite-part integral in (5.4.30) is that $\phi(x)$ satisfy a Hölder-continuous first derivative condition as in §5.2, which also guarantees that the first integral on the right side of (5.4.30) is, at most, weakly singular.

Integrating a finite-part integral by parts we get

$$\oint_a^b \frac{\phi(x)}{(x-s)^2} dx = \frac{\phi(a)}{a-s} - \frac{\phi(b)}{b-s} + \int_a^b \frac{\phi'(x)}{x-s} dx, \quad (5.4.31)$$

where $\phi(x) \in C^1[a, b]$ satisfies the Hölder condition. If we compare (5.4.31) and (5.4.29), we obtain

$$\frac{d}{ds} \oint_a^b \frac{\phi(x)}{x-s} dx = \oint_a^b \frac{\phi(x)}{(x-s)^2} dx,$$

which shows that differentiation can be carried out under the integral sign.

5.4.5. One-Sided Finite-Part Integrals. Consider the case when the integrand has a singularity at an endpoint of the interval $[a, b]$, that is, either $a \equiv s$ or $b \equiv s$. Then the finite-part of a first-order function $\phi(x) \in C^1[a, s]$ or $\phi(x) \in C^1[s, b]$ is defined, respectively, by

$$\oint_a^s \frac{\phi(x)}{x-s} dx = \int_a^s \frac{\phi(x) - \phi(s)}{x-s} dx + \phi(s) \oint_a^s \frac{dx}{x-s} \quad (5.4.32)$$

or

$$\oint_s^b \frac{\phi(x)}{x-s} dx = \int_s^b \frac{\phi(x) - \phi(s)}{x-s} dx + \phi(s) \oint_s^b \frac{dx}{x-s}, \quad (5.4.33)$$

where

$$\int_a^s \frac{dx}{x-s} = \text{finite part of } [\ln |x-s|]_a^s = -\ln |a-s|,$$

or

$$\int_s^b \frac{dx}{x-s} = \text{finite part of } [\ln |x-s|]_s^b = \ln |b-s|,$$

If $\phi(x) \notin C^1$, a sufficient condition for the existence of the finite-part integrals in (5.4.32) and (5.4.33) is that $\phi(x) \in C^0$ and satisfies a Hölder condition. If we use (5.4.32) and (5.4.33) to derive (5.4.26), we find that finite-part integrals exist iff the function $\phi(x)$ is continuous at the singular point s .

Similarly, the second-order one-sided finite-part integral of a function $\phi(x) \in C^2$ is given by

$$\begin{aligned} \int_a^s \frac{\phi(x)}{(x-s)^2} dx &= \int_a^s \frac{\phi(x) - \phi(s) - (x-s)\phi'(s)}{(x-s)^2} dx \\ &+ \phi(s) \int_a^s \frac{dx}{(x-s)^2} + \phi'(s) \int_a^s \frac{dx}{x-s}, \end{aligned} \quad (5.4.34)$$

or

$$\begin{aligned} \int_s^b \frac{\phi(x)}{(x-s)^2} dx &= \int_s^b \frac{\phi(x) - \phi(s) - (x-s)\phi'(s)}{(x-s)^2} dx \\ &+ \phi(s) \int_s^b \frac{dx}{(x-s)^2} + \phi'(s) \int_s^b \frac{dx}{x-s}, \end{aligned} \quad (5.4.35)$$

according as the singularity is at the endpoint b or the endpoint a of the interval $[a, b]$. In these cases then

$$\int_a^s \frac{dx}{(x-s)^2} = \text{finite part of } \left[-\frac{1}{x-s} \right]_a^s = \frac{1}{a-s},$$

or

$$\int_s^b \frac{dx}{(x-s)^2} = \text{finite part of } \left[-\frac{1}{x-s} \right]_s^b = \frac{1}{s-b},$$

respectively. If $\phi(x) \notin C^2$, a sufficient condition for the existence of the finite-part integrals in (5.4.34) and (5.4.35) is that $\phi(x) \in C^1$ and satisfy a Hölder condition. If we use (5.4.32) and (5.4.33) to derive (5.4.26), we find that finite-part integrals exist iff the function $\phi'(x)$ is continuous at the singular point s .

EXAMPLE 5.4.5. First, we define the Hadamard transform $H_2[\phi]$ for a function $\phi(x)$ as

$$H_2[\phi] = \int_0^1 \frac{\phi(x)}{(x-s)^2} dx, \quad 0 < s < 1. \quad (5.4.36)$$

Notice that this transform is the integral $I_{2,\nu}$. The results, given in Table 5.4.5, hold for various choices of the function ϕ .

Note that if the function $\phi(x) \in C^2[a, b]$ satisfies a Hölder-continuous second-derivative condition, then Hadamard's second-order two-sided finite-part integrals contain the singular part $\frac{1}{(x-s)^3}$ and can be defined as above (see Ioakimidas 1988, for details). This concept can be generalized further, but we shall not go into this generalization. Kutt (1975) contains weights w_i to 30S* for the equally spaced rule

$$\oint_0^1 \frac{f(x)}{x^4} dx \approx \sum_{i=1}^n w_i f\left(\frac{i}{n}\right), \quad n = 3(1)20,$$

and the nodes x_i and weights w_i to 30S for the Gauss-type quadrature rule

$$\oint_0^1 \frac{f(x)}{x^4} dx \approx \sum_{i=1}^n w_i f(x_i), \quad n = 2(1)20,$$

for $\lambda = 1, 4/3, 3/2, 5/3, 2, 3, 4, 5$. This work also contains weights for computation of the finite-part integrals of the form

$$\oint_0^1 \frac{f(x)}{(x-s)^4} dx, \quad \lambda = 2, 3, 4, 5$$

for the equally spaced case. ■

5.5. Computer-Aided Derivations

We will consider Cauchy p.v. integrals and the related hypersingular (finite part) integrals of the form

$$I(y) = \oint_a^b w(x) \frac{g(x)}{x-y} dx, \quad a < y < b, \quad (5.5.1)$$

$$J_p(y) = \oint_a^b w(x) \frac{g(x)}{(x-y)^p} dx, \quad a < y < b, \quad p = 1, 2, \dots \quad (5.5.2)$$

where $J_1(y) \equiv I(y)$. First, we give Mathematica code for the Gauss-Chebyshev and Gauss-Legendre rules; then we consider the problem where the singular point y coincides with a node, which leads to the computation of the related p.v. integral $q_0(y)$:

*'S' means 'significant digits'.

Table 5.4.5.

$\phi(s)$	$H_2[\phi]$
s^ν (ν rational)	$-\pi\nu s^{\nu-1} \cot \pi\nu - \frac{1}{1-s} - \nu \sum_{n=0}^{\infty} \frac{s^n}{n-\nu+1}$
s^m (m integer)	$\frac{s^{m-1}}{1-s} + ms^{m-1} \ln \frac{1-s}{s}$ $+ \sum_{j=2}^m \frac{\binom{m}{j} s^{m-j} [(1-s)^{j-1} - (-s)^{j-1}]}{j-1}$
$[s(1-s)]^{3/2}$	$\frac{\pi}{2} \left[\frac{3}{4} - 6s(1-s) \right]$
$\frac{1}{2} + \frac{s-c}{2 s-c }$	$\frac{1}{s-1} + \frac{1}{c-s}$
$\frac{1}{2} [c + (1-2c)s + s-c]$	$(c-1) \ln s - c \ln 1-s + \ln s-c $
$\frac{1}{2} + \frac{1}{4\epsilon} [s-c+\epsilon + s-c-\epsilon]$	$\frac{1}{s-1} + \frac{1}{2\epsilon} \ln \left \frac{s-c-\epsilon}{s-c+\epsilon} \right $
$\frac{3}{4} (s-c)^2 - \frac{1}{4} (s-c) s-c $ $+ \frac{1}{2} (s-c) (c^2 + 2c - 1)$ $+ \frac{1}{2} c (c^2 - 1)$	$c + 1 + \left(s + \frac{c^2}{2} - \frac{1}{2} \right) \ln 1-s $ $+ (s-c) \ln s-c $ $- \left(2s + \frac{c^2}{2} - c - \frac{1}{2} \right) \ln s $
$\sin \pi s$	$-\pi \sin \pi s [\text{Si}(\pi(1-s)) + \text{Si}(\pi s)]$ $+ \pi \cos \pi s [\text{Ci}(\pi s) - \text{Ci}(\pi(1-s))]$

$$q_0(y) = \int_a^b w(x) \frac{p_n(x)}{x-y} dx, \quad a < y < b, \quad (5.5.3)$$

where $p_0(x) \equiv 1$, and $p_n(x)$ denotes the polynomial whose roots are the nodes of the quadrature rule, i.e., $p_n(x) \equiv T_n(x)$ or $P_n(x)$ for the Gauss-Chebyshev or the Gauss-Legendre rule, respectively.

For the Cauchy p.v. integral (5.5.1) we consider the singularity at $x = y$. Assuming that $g \in C^1[a, b]$, we rewrite (5.5.1) by using (5.5.3) as

$$I(y) = \int_a^b w(x) \frac{g(x) - g(y)}{x-y} dx + q_0(y) g(y), \quad (5.5.4)$$

where the integral is now regular. In the case of $J_p(y)$ we write (5.5.2) as an appropriate derivative of $I(y)$:

$$J_p(y) = \frac{1}{(p-1)!} \frac{d^{p-1}}{dy^{p-1}} I(y), \quad p = 1, 2, \dots \quad (5.5.5)$$

We then use an interpolatory or Gaussian rule of the general form

$$\int_a^b w(x) f(x) dx = \sum_{k=1}^n w_{k,n} f(x_{k,n}) + E_n, \quad (5.5.6)$$

where $x_{k,n}$ denote the nodes, $w_{k,n}$ the related weights, and E_n the error term. Ioakimidis (1992) has provided Mathematica code to derive quadrature rules for singular and hypersingular integrals. The results are as follows.

5.5.1. Gauss-Chebyshev Rule. For the classical Gauss-Chebyshev rule we have $w(x) = \sqrt{1-x^2}$, and

$$\int_{-1}^1 \sqrt{1-x^2} f(x) dx = \sum_{k=1}^n w_{k,n} f(x_{k,n}) + E_n, \quad (5.5.7)$$

where $q_0(y) = -\pi y$, and

$$x_{n,k} = \cos \frac{(2k-1)\pi}{2n}, \quad w_{k,n} = \frac{(1-x_{n,k}^2)\pi}{n}, \quad k = 1, 2, \dots, n. \quad (5.5.8)$$

Then for $n = 3$ and $p = 1$:

$$I(y) = \pi \left(\frac{0.0833333 g(-0.866025)}{-0.866025 - y} - \frac{g(0)}{3y} + \frac{0.0833333 g(0.866025)}{0.866025 - y} + \frac{(-0.75 + 3.75y^2 - 3y^4) g(y)}{-2.25y + 3y^3} \right);$$

for $n = 3$ and $p = 2$:

$$I(y) = \pi \left(\frac{0.0833333 g(-0.866025)}{(-0.866025 - y)^2} + \frac{g(0)}{3y^2} + \frac{0.0833333 g(0.866025)}{(0.866025 - y)^2} + \frac{(-1.6875 - 1.6875y^2 + 9y^4 - 9y^6) g(y)}{y^2 (-2.25 + 3y^2)^2} + \frac{(-0.75 + 3.75y^2 - 3y^4) g'(y)}{-2.25y + 3y^3} \right);$$

and for $n = 3$ and $p = 3$:

$$I(y) = \frac{\pi}{2} \left(\frac{0.166667 g(-0.866025)}{(-0.866025 - y)^3} - \frac{2g(0)}{3y^3} + \frac{0.166667 g(0.866025)}{(0.866025 - y)^3} + \frac{(-7.59375 + 30.375y^2 - 20.25y^4 + 27y^6) g(y)}{y^2 (-2.25 + 3y^2)^2 (-2.25y + 3y^3)} + \frac{(-3.375 - 3.375y^2 + 18y^4 - 18y^6) g'(y)}{y^2 (-2.25 + 3y^2)^2} + \frac{(-0.75 + 3.75y^2 - 3y^4) g''(y)}{-2.25y + 3y^3} \right).$$

5.5.2. Gauss-Legendre Rule. For the classical Gauss-Chebyshev rule we have $w(x) = 1$, and

$$\int_{-1}^1 f(x) dx = \sum_{k=1}^n w_{k,n} f(x_{k,n}) + E_n, \quad (5.5.9)$$

where $q_0(y) = \log\left(\frac{1-y}{1+y}\right)$, and $x_{n,k}$ are the zeros of the Legendre polynomials $P_n(x)$ and the weights $w_{k,n}$ are given by

$$w_{k,n} = \frac{2 \left(1 - x_{n,k}^2\right)}{(n+1)^2 P_{n+1}'(x_{k,n})}, \quad k = 1, 2, \dots, n. \quad (5.5.10)$$

Then for $n = 4$ and $p = 1$:

$$\begin{aligned} I(y) = & \frac{0.347855 g(-0.861136)}{-0.861136 - y} + \frac{0.652145 g(-0.339981)}{-0.339981 - y} \\ & + \frac{0.652145 g(0.339981)}{0.339981 - y} + \frac{0.347855 g(0.861136)}{0.861136 - y} \\ & + \frac{\left(-1.04762y + 2y^3 + (0.0857143 - 0.857143 y^2 + y^4) \log \frac{1-y}{1+y}\right) g(y)}{0.0867143 - 0.857143 y^2 + y^4}; \end{aligned}$$

and for $n = 4$ and $p = 2$:

$$\begin{aligned} I(y) = & \frac{0.347855 g(-0.861136)}{(-0.861136 - y)^2} + \frac{0.652145 g(-0.339981)}{(-0.339981 - y)^2} \\ & + \frac{0.652145 g(0.339981)}{(0.339981 - y)^2} + \frac{0.347855 g(0.861136)}{(0.861136 - y)^2} \\ & + \frac{0.10449 g(y)}{(1-y)(1+y) (0.0857143 - 0.857143 y^2 + y^4)^2} \\ & + \frac{\left(-1.04762y + 2y^3 + (0.0857143 - 0.857143 y^2 + y^4) \log \frac{1-y}{1+y}\right) g'(y)}{0.0867143 - 0.857143 y^2 + y^4}. \end{aligned}$$

5.5.3. Singular Point as a Node. In the case of the Gauss-Legendre quadrature rule, if $y = x_{m,n}$ ($m = 1, 2, \dots, n$), we have (Ioakimidis and Theocaris 1977)

$$\begin{aligned} I(x_{m,n}) &= \int_{-1}^1 \frac{g(x)}{x - x_{m,n}} dx \\ &= \sum_{\substack{k=1 \\ k \neq m}}^n w_{k,m} \frac{g(x_{k,m})}{x_{k,n} - x_{k,m}} + w_{m,n} g'(x_{m,n}) + w_{m,n} g(x_{m,n}) + E_n, \end{aligned} \quad (5.5.11)$$

where the new weights $w_{m,n}$ are given by

$$w_{m,n} = -2 \frac{Q_{n-1}(x_{m,n})}{P_{n-1}(x_{m,n})} - (n+1) w_{m,n} \frac{x_{m,n}}{1-x_{m,n}^2}, \quad (5.5.12)$$

and $Q_n(x)$ denotes the classical Legendre function of the second kind which is defined by (Abramowitz and Stegun 1968, p. 334)

$$Q_n(x) = \frac{1}{2} P_n(x) \ln \frac{1+x}{1-x} - \sum_{m=1}^n \frac{1}{m} P_{m-1}(x) P_{n-m}(x).$$

While using Mathematica, we can obtain the form of the Gauss-Legendre quadrature rule for $y = x_{m,n}$ by means of a limiting process for a particular value of m . Thus, the results for $n = 4$ nodes and $p = 1$ (Cauchy singular integrals) with the Gauss-Legendre rule for all four nodes $x_{k,4}$, as given below, also contain analogous results for the first node $x_{1,4}$ in the case when $p = 2$ and $p = 3$ (hypersingular integrals). This gives the values of $w_{m,n}$ for $p = 1$, which match the values given by (5.5.12). The results are:

$$\begin{aligned} \lim_{y \rightarrow x_{1,4}} I(y) &= -0.201974 g(-0.861136) - 0.542949 g(-0.339981) \\ &\quad - 1.25135 g(0.339981) - 0.599181 g(0.861136) + 0.347855 g'(0.861136); \\ \lim_{y \rightarrow x_{2,4}} I(y) &= 0.599181 g(-0.861136) + 1.25135 g(-0.339981) \\ &\quad + 0.542949 g(0.339981) + 0.201974 g(0.861136) + 0.347855 g'(-0.861136); \\ \lim_{y \rightarrow x_{3,4}} I(y) &= -0.289609 g(-0.861136) - 0.95909 g(-0.339981) \\ &\quad - 0.126911 g(0.339981) + 0.667469 g(0.861136) + 0.652145 g'(0.339981); \\ \lim_{y \rightarrow x_{4,4}} I(y) &= -0.667469 g(-0.861136) + 0.126911 g(-0.339981) \\ &\quad + 0.95909 g(0.339981) + 0.289609 g(0.861136) + 0.652145 g'(-0.339981). \end{aligned}$$

For the hypersingular cases for $p = 2$:

$$\begin{aligned} \lim_{y \rightarrow x_{1,4}} I(y) &= 0.117272 g(-0.861136) + 0.452036 g(-0.339981) \\ &\quad + 2.4011 g(0.339981) - 10.709 g(0.861136) - 0.599181 g'(0.861136) \\ &\quad + 0.173927 g''(0.861136); \end{aligned}$$

and for $p = 3$:

$$\begin{aligned} \lim_{y \rightarrow x_{1,4}} I(y) &= \frac{1}{2} [-0.136183 g(-0.861136) - 0.752693 g(-0.339981) \\ &\quad - 9.21452 g(0.339981) - 41.4667 g(0.861136) - 0.599181 g''(0.861136) \\ &\quad + 2(-10.709 g'(0.861136) - 0.173927 g(0.861136)) \\ &\quad + 0.463806 g(0.861136)]. \end{aligned}$$

Ioakimidis and Theocaris (1977) have developed a Mathematica procedure, called PVI, that uses the definition

$$\oint_a^b \frac{g(x)}{x-y} dx = \lim_{\varepsilon \rightarrow 0} \left[\int_a^{y-\varepsilon} \frac{g(x)}{x-y} dx + \int_{y+\varepsilon}^b \frac{g(x)}{x-y} dx \right], \quad (5.5.13)$$

where $\varepsilon > 0$, and $a < y < b$, and computes the function $q_0(y)$ for the Gauss-Legendre, which is given by

$$q_0(y) = \oint_{-1}^1 \frac{1}{x-y} dx = \log \frac{1-y}{1+y}, \quad -1 < y < 1; \quad (5.5.14)$$

it also computes some other complicated cases of Cauchy singular integrals, e.g., $g(x) = x^m$, $g(x) = e^{-x}$, or $g(x) = \cos x$ for $[a, b] \equiv [-1, 1]$. The latter two cases involve the exponential integral $\text{Ei}(x)$ and the sine and cosine integrals $\text{Si}(x)$ and $\text{Ci}(x)$. Ashley and Landahl (1985) have studied the case of Mangler-type p.v. hypersingular integrals ($p = 2$).

Although Mathematica is useful in such research, care must be taken to avoid misleading results. Thus, in the case of Gauss-Chebyshev rule for Cauchy p.v. integrals, there is a region of instability near the origin $y = 0$; also, if we generate the formula for the Gauss-Jacobi rule for Cauchy p.v. integrals with $w(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$, and $[a, b] \equiv [-1, 1]$, more serious problems arise which are related to the computation of the auxiliary function $q_0(y)$ (see [Gautschi and Wimp 1987](#), where these problems are investigated in detail). Mathematica fails to compute $q_0(y)$ with the Jacobi weight function (according to Ioakimidis and Theocaris). The Mathematica package `CauchyPrincipalValue.m` is sometimes useful for Cauchy p.v. integrals.

6

Fourier Integrals and Transforms

Some quadrature rules for computing the Fourier integrals and Fourier transform are presented. The Fourier and Hartley transforms and discrete Fourier transform are discussed, and fast Fourier transform (FFT) and fast Hartley transform (FHT) are presented together with computer codes for their evaluation.

6.1. Fourier Transforms

We will consider the Fourier integrals of the form

$$I = \frac{1}{\pi} \int_0^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos \omega(x - t) dt, \quad f \in R(-\infty, \infty), \quad (6.1.1)$$

where ω is the angular frequency. The inner integral in (6.1.1) with respect to t is absolutely and uniformly convergent for all real x and ω . If the function f is of bounded variation on an interval $[a, b]$ and if $a < x < b$, then the integral (6.1.1) has the value $I = \frac{1}{2} [f(x + 0) + f(x - 0)]$; but if f is of bounded variation and $f \in C[a, b]$, then the integral (6.1.1) has the value $I = f(x)$, and the double integral (6.1.1) converges uniformly to $f(x)$ with respect to x in any closed interior subset of $[a, b]$. Assuming that the function f satisfies the Dirichlet's conditions, that is,

- (i) f has only a finite number of extrema in the interval (a, b) ;
- (ii) has only a finite number of finite discontinuities in this interval;
- (iii) for each point $x \in [a, b]$ the finite limits $f(x+)$ and $f(x-)$ exist, the relation $f(x) = \frac{1}{2} [f(x + 0) + f(x - 0)]$ holds for all x ; and
- (iv) $\int_a^b |f(x)| dx < +\infty$,

we will take $f(x)$ to be the value of the integral (6.1.1). Then we can define the Fourier transform by first considering the Fourier representation of f which is given by

$$\begin{aligned}
 f(x) &= \frac{1}{\pi} \int_0^\infty \int_{-\infty}^\infty f(t) [\cos \omega x \cos \omega t + \sin \omega x \sin \omega t] dt d\omega \\
 &= \frac{1}{\pi} \int_0^\infty \int_{-\infty}^\infty f(t) \cos \omega(x-t) dt d\omega \\
 &= \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^\infty f(t) [e^{i\omega(x-t)} + e^{-i\omega(x-t)}] dt d\omega \\
 &= \frac{1}{2\pi} \int_{-\infty}^\infty \int_{-\infty}^\infty f(t) e^{i\omega(x-t)} dt d\omega \\
 &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{i\omega x} d\omega \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty f(t) e^{-i\omega t} dt. \tag{6.1.2}
 \end{aligned}$$

This is known as the *Fourier complex formula*, which leads to the definition of three Fourier transform pairs, as follows. Let $f \in L_2(-\infty, \infty)$. Then

FOURIER COMPLEX TRANSFORM PAIR. $\mathcal{F}f(x) = F(\omega)$ of $f(x)$ and its inverse are defined as

$$\mathcal{F}\{f(x)\} \equiv F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty f(t) e^{-i\omega t} dt, \tag{6.1.3a}$$

$$\mathcal{F}^{-1}\{F(\omega)\} \equiv f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty F(\omega) e^{i\omega x} d\omega, \tag{6.1.3b}$$

where $F \in L_2(-\infty, \infty)$, and ω denotes the radial frequency. The factor $1/\sqrt{2\pi}$ in both definitions makes $|F(\omega)|^2$ proportional to the energy density of F at frequency ω in the same ratio $|f(x)|^2$ is proportional to the energy density at time x . Some authors use the definition of $F(\omega)$ without this factor and place $1/(2\pi)$ with the definition of $f(t)$. Others use the definition $F(\alpha) = \int_{-\infty}^\infty f(t) e^{-2\pi i \alpha t} dt$, where α is the frequency which is related to the radian frequency by $\omega = 2\pi\alpha$; this definition becomes useful in computation where α is known. The complex Fourier transform pairs (6.1.3a,b) are also known as Plancherel theorem.

Let the delta function $\delta_a(x)$, which has a unit mass at a , be defined by $\delta_a(x) = \frac{d}{dx} H_a(x)$, where $H_a(x)$ is the Heaviside function $H_a(x) = \begin{cases} 1, & x > a, \\ 0, & x \leq a. \end{cases}$ Let T_a denote the translation, and $\delta = \delta_0 = \lim_{n \rightarrow \infty} n \chi_{[0, 1/n)}(x)$, where $\chi_{[0, 1/n)}(x)$ is the characteristic function of the interval $[0, 1/n)$.

EXAMPLE 6.1.1 Some useful complex Fourier transforms are given below.

$$\mathcal{F}\{\delta_a(x)\} = \frac{1}{\sqrt{2\pi}} e^{-ia\omega},$$

$$\mathcal{F}\left\{\sum_k \delta(t - 2\pi k)\right\} = \frac{1}{\sqrt{2\pi}} \sum_k \delta(\omega - n),$$

$$\mathcal{F}\{x^k e^{-i\sigma x}\} = \sqrt{2\pi} i^k \delta^{(k)}(\omega + \sigma),$$

$$\mathcal{F}\{e^{-|x|/b}\} = \sqrt{\frac{2}{\pi}} \frac{b}{1 + b^2\omega^2},$$

$$\mathcal{F}\{\text{p.v.} \frac{1}{x}\} = -i \sqrt{\frac{\pi}{2}} \operatorname{sgn} \omega,$$

$$\mathcal{F}\left\{\sum_n a_n e^{inx}\right\} = \sqrt{2\pi} \sum_n a_n \delta(\omega - n),$$

$$\mathcal{F}\{\chi_{[r,s)}(x)\} = \frac{e^{-i\omega(r+s)/2}}{\sqrt{2\pi}} \frac{\sin((s-r)\omega/2)}{\omega/2},$$

$$\mathcal{F}\{\chi_{[0,1)}(x)\} = \frac{e^{-i\omega/2}}{\sqrt{2\pi}} \frac{\sin(\omega/2)}{\omega/2} = \frac{e^{-i\omega/2}}{\sqrt{2\pi}} \operatorname{sinc}\left(\frac{\omega}{2\pi}\right),$$

$$\mathcal{F}\{\chi_{[-1,1)}(x)\} = \sqrt{\frac{2}{\pi}} \frac{\sin \omega}{\omega} = \sqrt{\frac{2}{\pi}} \operatorname{sinc} \omega,$$

$$\mathcal{F}\left\{\sum_n a_n e^{inx} \chi_{[-\pi,\pi]}(x)\right\} = \sqrt{2\pi} \sum_n a_n \frac{\sin \pi(\omega - n)}{\pi(\omega - n)}. \blacksquare$$

FOURIER COSINE TRANSFORM PAIR. $F_c(\omega)$ of $f(x)$ and its inverse are defined as

$$\mathcal{F}_c\{f(x)\} \equiv F_c(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \cos(\omega t) dt, \quad (6.1.4a)$$

$$\mathcal{F}^{-1}\{F_c(\omega)\} \equiv f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_c(\omega) \cos(x\omega) d\omega. \quad (6.1.4b)$$

FOURIER SINE TRANSFORM PAIR. $F_s(\omega)$ of $f(x)$ and its inverse are defined as

$$\mathcal{F}_s\{f(x)\} \equiv F_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \sin(\omega t) dt, \quad (6.1.5a)$$

$$\mathcal{F}^{-1}\{F_s(\omega)\} \equiv f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_s(\omega) \sin(x\omega) d\omega. \quad (6.1.5b)$$

Let f and g belong to the class L_2 . Some properties of the complex Fourier transforms are:

$$(1) \mathcal{F}\{af(tx + bg(x))\} = aF(\omega) + bG(\omega) \quad (\text{Linearity});$$

$$(2) \mathcal{F}\{f(x - a)\} = e^{i\omega a} F(\omega) \quad (\text{Shifting});$$

$$(3) \mathcal{F}\{f(ax)\} = \frac{1}{|a|} F(\omega/a) \quad (\text{Scaling});$$

(4) $\mathcal{F}\{e^{iax}f(x)\} = F(\omega + a)$ (Modulation);

(5) The convolution (or Faltung) of $f(t)$ and $g(t)$ over $(-\infty, \infty)$ is defined by

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\eta)g(x - \eta) d\eta = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x - \eta)g(\eta) d\eta. \quad (6.1.6)$$

Let $F(\omega)$ and $G(\omega)$ be the Fourier transforms of $f(x)$ and $g(x)$, respectively. Then the inverse Fourier transform of $F(\omega)G(\omega)$ is

$$\mathcal{F}^{-1}\{F(\omega)G(\omega)\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\eta)g(x - \eta) d\eta,$$

and

$$\int_{-\infty}^{\infty} F(\omega)G(\omega) d\omega = \int_{-\infty}^{\infty} f(-\eta)g(\eta) d\eta.$$

PROPERTIES OF FOURIER SINE AND COSINE TRANSFORMS:

(1) $\mathcal{F}_c\{f(x)\} = F_c(\omega)$, $\mathcal{F}_s\{f(x)\} = F_s(\omega)$;

(2) $\mathcal{F}_c\{f(kx)\} = \frac{1}{k}F_c\left(\frac{\omega}{k}\right)$, $k > 0$;

(3) $\mathcal{F}_s\{f(kx)\} = \frac{1}{k}F_s\left(\frac{\omega}{k}\right)$, $k > 0$;

(4) $\mathcal{F}_c\{f(kx) \cos bx\} = \frac{1}{2k} \left[F_c\left(\frac{\omega + b}{k}\right) + F_c\left(\frac{\omega - b}{k}\right) \right]$, $k > 0$;

(5) $\mathcal{F}_c\{f(kx) \sin bx\} = \frac{1}{2k} \left[F_s\left(\frac{\omega + b}{k}\right) - F_s\left(\frac{\omega - b}{k}\right) \right]$, $k > 0$;

(6) $\mathcal{F}_s\{f(kx) \cos bx\} = \frac{1}{2k} \left[F_s\left(\frac{\omega + b}{k}\right) + F_s\left(\frac{\omega - b}{k}\right) \right]$, $k > 0$;

(7) $\mathcal{F}_s\{f(kx) \sin bx\} = \frac{1}{2k} \left[F_c\left(\frac{\omega - b}{k}\right) - F_c\left(\frac{\omega + b}{k}\right) \right]$, $k > 0$.

CONVOLUTION OF FOURIER SINE AND COSINE TRANSFORMS. Let $F_c(\omega)$ and $G_c(\omega)$ be the Fourier cosine transforms of $f(x)$ and $g(x)$, respectively, and let $F_s(\omega)$ and $G_s(\omega)$ be the Fourier sine transforms of $f(x)$ and $g(x)$, respectively. Then

$$\mathcal{F}_c^{-1}[F_c(\omega)G_c(\omega)] = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} g(\eta)[f(|x - \eta|) + f(x + \eta)] d\eta.$$

If $F_s(\omega)$, $F_c(\omega)$ and $G_s(\omega)$, $G_c(\omega)$ are the Fourier sine and cosine transforms of $f(x)$ and $g(x)$, respectively, then the following results hold:

$$(1) \int_0^{\infty} F_c(\omega) G_s(\omega) \sin \omega x d\omega = \frac{1}{2} \int_0^{\infty} g(\eta)[f(|x - \eta|) - f(x + \eta)] d\eta,$$

$$(2) \int_0^\infty F_s(\omega) G_c(\omega) \sin \omega x d\omega = \frac{1}{2} \int_0^\infty f(\eta) [g(|x - \eta|) - g(x + \eta)] d\eta,$$

$$(3) \int_0^\infty F_s(\omega) G_s(\omega) \cos \omega x d\omega \\ = \frac{1}{2} \int_0^\infty g(t) [H(t + x) f(t + x) + H(t - x) f(t - x)] dt \\ = \frac{1}{2} \int_0^\infty f(t) [H(t + x) g(t + x) + H(t - x) g(t - x)] dt;$$

$$(4) \int_0^\infty F_c(\omega) G_c(\omega) d\omega = \int_0^\infty f(\eta) g(\eta) d\eta = \int_0^\infty F_s(\omega) G_s(\omega) d\omega.$$

6.1.1. Use of Simpson's Rule. To compute the Fourier transform $F(\omega)$, defined by (6.1.3a), first we rewrite $f(t)$ defined by (6.1.3b) as

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty F(\omega) e^{-i\omega t} d\omega = \sqrt{\frac{2}{\pi}} \int_0^\infty \Re \{ F(\omega) e^{-i\omega t} \} d\omega. \quad (6.1.7)$$

We use Simpson's rule to yield

$$F(\omega) \approx \frac{h}{6} \sqrt{\frac{2}{\pi}} \left[f(0) + 4 \sum_{j=1}^{N/2} f_{2j-1} e^{i\omega t_{2j-1}} \right. \\ \left. + 2 \sum_{j=1}^{N/2-1} f_{2j} e^{i\omega t_{2j}} + f(Nh) e^{i\omega Nh} \right], \quad (6.1.8)$$

where $t_j = jh$, $f_j = f(t_j)$, h is the step size, and N is even. In the inversion process from $F(\omega)$ to $f(t)$ we start with a finite number of values $F(\omega_1), F(\omega_2), \dots, F(\omega_n)$. But the computer time depends on the value of n . In order to minimize computation it is always better to use the fewest of these values. But this choice is not simple, because choosing (ω_n) too low uses only a small portion of the spectrum and may miss its significant portion, while choosing these values too high may pick negligible frequency components and waste computation time. The problem of choosing the optimal frequency spectrum of an unknown output waveform is, therefore, difficult. As suggested by Meisel (1968), the solution is to sample less often at higher frequencies, thus choosing the sample logarithmically, i.e., using $\omega_0, K\omega_0, K^2\omega_0, \dots, K^n\omega_0$, where $K > 1$. Hence, we use an approximation that matches a quadratic to three points in every two adjacent intervals, with sampling points of $\omega_0, K\omega_0, K^2\omega_0, \dots, K^n\omega_0$, and require that

$$\int_{\omega_0}^{K^2\omega_0} F(\omega) d\omega = x F(\omega_0) + y F(K\omega_0) + z F(K^2\omega_0)$$

must be exact for $F(\omega) = 1, \omega, \omega^2$. This yields the set of simultaneous equations

$$x + y + z = \omega_0 (K^2 - 1), \\ x + Ky + K^2z = \frac{1}{2} \omega_0 (K^4 - 1), \\ x + K^2y + K^4z = \frac{1}{3} \omega_0 (K^6 - 1),$$

which are solved to give

$$\begin{aligned}x &= \frac{\omega_0}{6} (K^2 - 1) (K - 2), & y &= \frac{\omega_0}{6K} (k - 1)(k + 1)^3, \\z &= \frac{\omega_0}{6K} (K^2 - 1) (2K - 1).\end{aligned}$$

Hence, the Simpson's formula is

$$\int_{\omega_0}^{K^n \omega_0} F(\omega) d\omega \approx \frac{\omega_0}{6} \sum_{j=1}^{n/2} \left[K^{2j-2} (f_{2j-2} A_0 + f_{2j-1} A_1 + f_{2j} A_2) \right], \quad (6.1.9)$$

where

$$\begin{aligned}A_0 &= -(K - 2) (K^2 - 1), & A_1 &= \frac{(K - 1)(K + 1)^3}{K}, \\A_2 &= \frac{(K^2 - 1) (2K - 1)}{K}.\end{aligned}$$

The choice of K is made by taking $K = \left(\frac{\omega_{\max}}{\omega_0} \right)^{1/n}$, where the maximum frequency ω_{\max} is known. Note that $A_0 = 0$ if $K = 2$.

6.1.2. Uncertainty Principle. The Heisenberg uncertainty principle of quantum mechanics states that the product of the uncertainty in position and the uncertainty in momentum is always greater than or equal to a particular constant. This principle is also true for signal processing. It means that an accurate determination of the frequency content of a signal requires a long measuring time, or equivalently, a short-duration signal contains a wide range of frequencies. These facts are derived from the same inequality that relates the properties of a function $f(t)$ and its Fourier transform $F(\omega)$. Let Δt denote the uncertainty in time t and $\Delta\omega$ the uncertainty in the frequency ω of the signal. Then the uncertainty principle states that $\Delta t \cdot \Delta\omega \geq \frac{1}{2}$. This inequality cannot be improved unless some new definitions of frequency, time and uncertainty are introduced.

The Fourier transform $F(\omega)$ defined by (6.1.3a) is also known as the *spectral function* of f with pure harmonics $e_{\omega} \equiv e^{i\omega t}$ as the basis functions for the radian frequency ω . The value of $F(\omega)$ for a given ω may be regarded as the complex amplitude by which the frequency ω is present in the signal f . The oscillation impulse which shows up in the time interval $[t_0 - h, t_0 + h]$, $h > 0$, but is identically zero outside this interval and which has a frequency range $[\omega_0 - \delta, \omega_0 + \delta]$, where $\delta > 0$ is arbitrarily small, does not exist, since the Heisenberg uncertainty principle gives

$$\int_{-\infty}^{\infty} t^2 |f(t)|^2 dt \cdot \int_{-\infty}^{\infty} \omega^2 |F(\omega)|^2 d\omega \geq \frac{1}{4} \|f\|^4, \quad (6.1.10)$$

where $\|f\|^2 = (2\pi)^{-1} \int_{-\infty}^{\infty} |f(t)|^2 dt$. The first factor in (6.1.10) is a measure of the ‘speed’ of the graph of f over the t -axis, whereas the second factor is a measure of the ‘speed’ of the graph of F over the ω -axis. The inequality (6.1.10) implies that the graphs of f and F cannot simultaneously have a single peak at the origin. The equality in (6.1.10) holds only for $f(t) = e^{-ct^2}$, $c > 0$.

6.1.3. Short Time Fourier Transform. If the signal $f(t)$ is not a periodic function, the Fourier series representation of $f(t)$, which is the sum of sine and cosine functions (periodic themselves), will not represent the signal. By artificially extending the signal and requiring that f be continuous at the endpoints, we can make it periodic, and obtain its Fourier representation and Fourier transform. However, a better solution is the *windowed* or *short time Fourier transform* (WFT or STFT), which provides information about signals simultaneously in both the time domain and the frequency domain. We define the WFT by choosing a window function $g(t)$ which has a total mass 1, is centered about $t = 0$ and decays rapidly as $|t| \rightarrow \infty$. Consider two different signals $f_1(t)$ and $f_2(t)$ defined by

$$f_1(t) = \begin{cases} f(t), & 0 \leq t \leq 1, \\ 0, & \text{otherwise,} \end{cases} \quad f_2(t) = \begin{cases} f(t), & 1 \leq t \leq 2, \\ 0, & \text{otherwise,} \end{cases}$$

or $f_1(t) = f(t) u_1(t - \frac{1}{2})$, $f_2(t) = f(t) u_1(t - \frac{3}{2})$, where

$$u_T(t - s) = \begin{cases} 1, & s - T/2 \leq t \leq s + T/2, \\ 0, & \text{otherwise,} \end{cases}$$

or, more precisely, define

$$f_s(t) = f(t) g(t - s) = f(t) u_T(t - s) = \begin{cases} f(t), & s - T \leq t \leq s + T, \\ 0, & \text{otherwise,} \end{cases}$$

where the parameter T is the time delay. Then the Fourier transform of $f_s(t)$ is

$$\begin{aligned} F(s, \omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_s(t) e^{-i\omega t} dt \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) g(t - s) e^{-i\omega t} dt. \end{aligned} \quad (6.1.11)$$

The transform defined by (6.1.11) is known as the WFT or STFT of the function $g(t)$. A widely used window function, introduced by Gabor (1946), is

$$g(t) \equiv \mathcal{N}_{0,\sigma}(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/(2\sigma^2)}, \quad (6.1.12)$$

where σ is a fixed parameter. Then the corresponding WFT of a function f is defined by (6.1.11) is also called the *Gabor transform*. For the above function g the function

$F(\omega, s)$ defined by (6.1.11) represents the complex amplitude by which the pure harmonic $e^{i\omega t}$ is present in f during the short time interval $[t_0 - \delta, t_0 + \delta]$, $\delta > 0$.

Thus, using the WFT we can chop up the signal $f(t)$ into sections, and then analyze each section separately for its frequency data. If f has sharp corners, we window the input data in such a manner that the sections converge to zero at the endpoints (Kaiser 1994). This windowing setup requires a window function g that has far less contribution at the endpoints than in the middle. Hence, the window is effective in localizing the signal in time.

6.2. Interpolatory Rules for Fourier Integrals

In order to evaluate the Fourier transforms numerically, we can use quadrature rules to compute the Fourier integrals for $F(\omega)$, $F_c(\omega)$, and $F_s(\omega)$, defined by (6.1.3a), (6.1.4a), and (6.1.5a), respectively. But these rules are not useful for two reasons: (i) They and their error estimates are well known and have been extensively studied, and (ii) they all have one basic drawback in that they are obtained by replacing the integrands on the entire interval of integration (or any of its part) by an algebraic polynomial of low degree. As such they produce good accuracy only if the integrand is a smooth function that does not vary rapidly. However, two of the Fourier integrals contain integrands which are the product $f(t) \cos \omega t$ and $f(t) \sin \omega t$. If the parameter ω (which represents the angular frequency in radians per sec) is large, the integrand oscillates rapidly, which results in the value of the integral with admissible error even after taking a very large number of points in the quadrature rule even for a slowly varying function $f(t)$. This makes the computation very difficult and prone to large errors. A similar situation can also arise in the case of the integral for $F(\omega)$. We are, therefore, obliged to develop new formulas that take into account the large variations of ω . This is done by taking such factors as weight functions.

We will assume that the function $f(t) \rightarrow 0$ as $|t| \rightarrow \infty$ so fast that the convergence of the integrals $\int_0^\infty |f(t)| dt$ or $\int_{-\infty}^\infty |f(t)| dt$ is assured. For the sake of definiteness we also assume that the inequality $|f(t)| \leq A|t|^{-1-\varepsilon}$, $\varepsilon > 0$ holds for large values of t . Let $[a, b]$ denote an arbitrary finite interval and let $p(x) \in \mathcal{P}_n$. By using repeated integration by parts, we obtain

$$\begin{aligned} \int_a^b p(x) e^{i\omega b} dx &= e^{i\omega b} \left[-\frac{ip(b)}{\omega} + \frac{p'(b)}{\omega^2} + \frac{ip''(b)}{\omega^3} - \frac{p'''(b)}{\omega^4} - \dots \right] \\ &\quad - e^{i\omega a} \left[-\frac{ip(a)}{\omega} + \frac{p'(a)}{\omega^2} + \frac{ip''(a)}{\omega^3} - \frac{p'''(a)}{\omega^4} - \dots \right] \\ &= e^{i\omega(b+a)/2} \left\{ \left[-\frac{ip(b)}{\omega} + \frac{p'(b)}{\omega^2} + \frac{ip''(b)}{\omega^3} - \frac{p'''(b)}{\omega^4} - \dots \right] e^{i\omega(b-a)/2} \right. \\ &\quad \left. - \left[-\frac{ip(a)}{\omega} + \frac{p'(a)}{\omega^2} + \frac{ip''(a)}{\omega^3} - \frac{p'''(a)}{\omega^4} - \dots \right] e^{-i\omega(b-a)/2} \right\}. \end{aligned} \quad (6.2.1)$$

If we take $p(x)$ as a real polynomial, then equating the real and imaginary parts in (6.2.1) we get

$$\begin{aligned} \int_a^b p(x) \cos \omega x \, dx &= \cos \frac{\omega(b+a)}{2} \left\{ \left[\frac{p(b)+p(a)}{\omega} - \frac{p''(b)+p''(a)}{\omega^3} + \dots \right] \sin \frac{\omega(b-a)}{2} \right. \\ &\quad \left. + \left[\frac{p'(b)-p'(a)}{\omega^2} - \frac{p'''(b)-p'''(a)}{\omega^4} + \dots \right] \cos \frac{\omega(b-a)}{2} \right\} \\ &+ \sin \frac{\omega(b+a)}{2} \left\{ \left[\frac{p(b)-p(a)}{\omega} - \frac{p''(b)-p''(a)}{\omega^3} + \dots \right] \cos \frac{\omega(b-a)}{2} \right. \\ &\quad \left. - \left[\frac{p'(b)+p'(a)}{\omega^2} - \frac{p'''(b)+p'''(a)}{\omega^4} + \dots \right] \sin \frac{\omega(b-a)}{2} \right\}, \end{aligned} \quad (6.2.2)$$

$$\begin{aligned} \int_a^b p(x) \sin \omega x \, dx &= \sin \frac{\omega(b+a)}{2} \left\{ \left[\frac{p(b)+p(a)}{\omega} - \frac{p''(b)+p''(a)}{\omega^3} + \dots \right] \sin \frac{\omega(b-a)}{2} \right. \\ &\quad \left. + \left[\frac{p'(b)-p'(a)}{\omega^2} - \frac{p'''(b)-p'''(a)}{\omega^4} + \dots \right] \cos \frac{\omega(b-a)}{2} \right\} \\ &- \cos \frac{\omega(b+a)}{2} \left\{ \left[\frac{p(b)-p(a)}{\omega} - \frac{p''(b)-p''(a)}{\omega^3} + \dots \right] \cos \frac{\omega(b-a)}{2} \right. \\ &\quad \left. - \left[\frac{p'(b)+p'(a)}{\omega^2} - \frac{p'''(b)+p'''(a)}{\omega^4} + \dots \right] \sin \frac{\omega(b-a)}{2} \right\}. \end{aligned} \quad (6.2.3)$$

It is easy to see that the above results hold for any complex polynomial $p(x)$.

6.2.1. Spline Interpolatory Rules. This implies an algebraic interpolation when a specific interpolating polynomial is constructed for each subinterval, and the polynomials are chosen such that at the boundary points of two adjacent subintervals the corresponding polynomials and their derivatives up to a certain order possess the same values. We will derive the interpolation formulas for the Fourier cosine integral $F_c(\omega)$. We partition the interval $[0, \infty)$ into a finite number of subintervals at the points $0 = x_0 < x_1 < \dots < x_k < \dots$. Consider one of these subintervals $[x_k, x_{k+1}]$. Assuming that the function f is sufficiently smooth, on this subinterval we will interpolate the function f by an algebraic polynomial. For example, we choose the interpolation with respect to the values of the function; thus, on $[x_k, x_{k+1}]$ we take $n_k + 1$ arbitrarily spaced points $x_j^k, j = 0, 1, \dots, n_k$, such that $x_k \leq x_0^k < \dots < x_{n_k}^k \leq x_{k+1}$, and perform the interpolation with respect to the values $f(x_j^k) = f_j^{(k)}$

by means of a polynomial $P_k(x)$ of degree n_k :

$$\begin{aligned} P_k(x) &= \sum_{j=0}^{n_k} \frac{\pi_k(x)}{(x - x_j^k) \pi'_k(x_j^k)} f_j^{(k)} = \sum_{j=0}^{n_k} l_j^{(k)}(x) f_j^{(k)}, \\ \pi_k(x) &= (x - x_0^k) \dots (x - x_{n_k}^k), \\ f(x) &= P_k(x) + e_k(x). \end{aligned}$$

Now, consider an integral of the form (6.1.4a) over the subinterval $[x_k, x_{k+1}]$, where we will ignore the constant factor $\sqrt{2/\pi}$ for now, and replace the function $f(x)$ on this subinterval by the interpolating polynomial $P_k(x)$. Then we get

$$\int_{x_k}^{x_{k+1}} f(t) \cos \omega t dt \approx \int_{x_k}^{x_{k+1}} P_k(t) \cos \omega t dt = \sum_{j=0}^{n_k} f_j^{(k)} \int_{x_k}^{x_{k+1}} l_j^{(k)}(t) \cos \omega t dt.$$

Summing such equations over all subintervals, we obtain the following approximate formula for the Fourier cosine integral:

$$F_c(\omega) = \int_0^\infty f(t) \cos \omega t dt \approx \sum_{k=0}^\infty \sum_{j=0}^{n_k} f_j^{(k)} \int_{x_k}^{x_{k+1}} l_j^{(k)}(t) \cos \omega t dt. \quad (6.2.4)$$

Each integral under the double summation in (6.2.4) can be computed from formula (6.2.2).

Since $e_k = f(x) - P_k(x)$ denotes the error of interpolation in the subinterval $[x_k, x_{k+1}]$, the total error in (6.2.4) is

$$E_c(\omega) = \sum_{k=0}^\infty \int_{x_k}^{x_{k+1}} |e_k(t)| dt,$$

which leads to the error estimate

$$|E_c(\omega)| \leq \sum_{k=0}^\infty \int_{x_k}^{x_{k+1}} |e_k(t)| dt. \quad (6.2.5)$$

Here we assume that the right side of the inequality (6.2.5) has a finite value. This value depends on the choice of the points x_k , the numbers n_k , the interpolation points $x_j^{(k)}$, the behavior of the function f , in particular whether it has derivatives of sufficiently large order, and the rate at which these derivatives approach zero as $t \rightarrow \infty$. Note that the estimate (6.2.5) is in general very complicated and has only theoretical value. Some specific cases are given below.

CASE 1. LINEAR INTERPOLATION. Let the interval $[0, \infty)$ be partitioned into equal subintervals of length $h > 0$ by the points $x_k = kh$, $k = 0, 1, 2, \dots$, and let

the values of the function f at these points be denoted by $f(x_k) = f(kh) = f_k$. The linear interpolation of f with respect to the values at the two endpoints of the subinterval $[kh, (k+1)h]$ is given by (1.5.1), which represents a trapezoidal type rule. If $f \in C^2[kh, (k+1)h]$, the error $E_k(x, f)$ is given by (1.5.2). If we multiply both sides of (1.5.2) by $\cos \omega x$ and integrate over the subinterval $[kh, (k+1)h]$, we get

$$\begin{aligned} & \int_{kh}^{(k+1)h} \left[\frac{x - kh}{h} f_{k+1} - \frac{x - (k+1)h}{h} f_k \right] \cos \omega x \, dx \\ &= \frac{1}{\omega} \left[f_{k+1} \sin \omega(k+1)h - f_k \sin \omega kh \right] \\ & \quad + \frac{1}{\omega^2 h} (f_{k+1} - f_k) [\cos \omega(k+1)h - \cos \omega h], \end{aligned}$$

which leads to

$$\begin{aligned} F_c(\omega) &= \int_0^\infty f(t) \cos \omega t \, dt \\ &= \frac{1 - \cos \omega h}{\omega^2 h} \left[f_0 + 2 \sum_{k=1}^\infty f_k \cos \omega kh \right] + E_c(\omega), \end{aligned} \quad (6.2.6a)$$

where

$$\begin{aligned} E_c(\omega) &= h^3 \int_0^1 \int_0^1 [(\xi - \tau)U(\xi - \tau) - \xi(1 - \tau)] \\ & \quad \times \sum_{k=0}^\infty f''(kh + \tau h) \cos \omega(kh + \xi h) \, d\tau \, d\xi. \end{aligned}$$

This yields the error bound

$$|E_c(\omega)| \leq \frac{h^3}{12} \sum_{k=0}^\infty |f''(kh + \theta h)|, \quad 0 < \theta < 1. \quad (6.2.6b)$$

Now, since this estimate depends on f'' , suppose that f'' is such that $|f''(x)| \leq \frac{B}{(a+x)^\nu}$, $a > 0$, $\nu > 1$. Then

$$\sum_{k=0}^\infty |f''(kh + \tau h)| \leq B \sum_{k=0}^\infty (a + kh + \tau h)^{-\nu} < B \sum_{k=0}^\infty (a + kh)^{-\nu}.$$

If h and a are preassigned, the value of the last sum is computed. Another simpler but less accurate estimate is obtained if

$$\int_k^{k+1} (a + ht)^{-\nu} \, dt < (a + kh)^{-\nu} < \int_{k-1}^k (a + ht)^{-\nu} \, dt;$$

in this case we have

$$|E_c(\omega)| \leq \frac{h^2}{12} \left[\frac{1}{(\omega - 1)^{a\omega-1}} + \frac{h}{\omega^2} \right]. \quad (6.2.6c)$$

The estimate (6.2.6b) can be used for getting estimates of different types, which are useful in certain cases. For example, in the case when f is a monotone or piecewise monotone function, we have

$$|E_c(\omega)| \leq \frac{h^2}{2} V_0^\infty \{f'(t)\},$$

where $V_0^\infty \{f\}$ denotes the (total) variation of f on the interval $[0, \infty)$. For the FOURIER SINE TRANSFORM we obtain the following result in terms of the values of the function f at the points $x_k = kh, k = 0, 1, \dots$:

$$\begin{aligned} F_s(\omega) &= \frac{1}{\omega} \left(1 - \frac{\sin \omega h}{\omega h} \right) f_0 \\ &\quad + 2 \frac{1 - \cos \omega h}{\omega^2 h} \sum_{k=1}^{\infty} f_k \sin \omega kh + E_s(\omega), \end{aligned} \quad (6.2.7a)$$

$$\begin{aligned} E_s(\omega) &= h^3 \int_0^1 \int_0^1 [(\xi - \tau)U(\xi - \tau) - \xi(1 - \tau)] \\ &\quad \times \sum_{k=0}^{\infty} f''(kh + \tau h) \sin \omega(kh + \xi h) d\tau d\xi. \end{aligned} \quad (6.2.7b)$$

The error $E_s(\omega)$ is similar to $E_c(\omega)$ except that it differs in the function $\cos \omega(kh + \xi h)$ which is replaced by $\sin \omega(kh + \xi h)$. Thus, if the function $f \in C^2[0, \infty]$ that decreases sufficiently rapidly as $x \rightarrow \infty$, we get

$$|E_s(\omega)| \leq \frac{h^3}{12} \sum_{k=0}^{\infty} |f''(kh + \theta h)|, \quad 0 < \theta < 1, \quad (6.2.7c)$$

$$|E_s(\omega)| \leq \frac{h^2}{2} V_0^\infty \{f'(t)\}. \quad (6.2.7d)$$

In the case when $|f''(x)| \leq B(a + x)^\nu$, $a > 0$, $\nu > 1$, the error estimate $E_s(\omega)$ has the same bounds as in (6.2.6c).

For the FOURIER COMPLEX TRANSFORM, we have the following representation in terms of the values of f at the points $x_k = kh, k = 0, \pm 1, \pm 2, \dots$:

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{iht} = 2 \frac{1 - \cos \omega h}{\omega^2 h} \sum_{k=-\infty}^{\infty} f_k e^{-i\omega kh} + E(\omega), \quad (6.2.8a)$$

$$\begin{aligned} E(\omega) &= h^3 \int_0^1 \int_0^1 [(\xi - \tau)U(\xi - \tau) - \xi(1 - \tau)] \\ &\quad \times \sum_{k=-\infty}^{\infty} f''(kh + \tau h) e^{-\omega(k+\xi)h} d\tau d\xi. \end{aligned} \quad (6.2.8b)$$

Thus, if the function $f \in C^2[0, \infty]$ that decreases sufficiently rapidly as $x \rightarrow \infty$, we get the same bounds for $E(\omega)$ as in (6.2.7c) and (6.2.7d); and in the case when $|f''(x)| \leq B(a+x)^\nu$, $a > 0$, $\nu > 1$, the error estimate $E(\omega)$ has the same bounds as in (6.2.6c).

CASE 2. QUADRATIC INTERPOLATION. If we interpolate the function f in the interval $[kh, (k+2)h]$ of length $2h$ with respect to the values f_k, f_{k+1} , and f_{k+2} at the points $kh, (k+1)h$, and $(k+2)h$ with a polynomial $P_2(x)$ of degree 2, then the parabolic interpolation is given by (1.5.3), and the related error by (1.5.5) or (1.5.6). If we multiply both sides of (1.5.3) by $\cos \omega x$, integrate over the interval $[x_k, x_{k+2}]$, and sum the result term-by-term over the even values of k , $k = 0, 2, 4, \dots$, then we obtain the following representation of the Fourier cosine transform in terms of the values $f_k, k = 0, 1, \dots$:

$$\begin{aligned} F_c(\omega) &= \int_0^\infty f(x) \cos \omega x \, dx \\ &= a_2 f_0 + c_2 \sum_{k=0}^\infty f_{2k+1} \cos(2k+1)\beta + 2a_2 \sum_{k=0}^\infty f_{2k+1} \cos 2k\beta + E_c, \end{aligned} \quad (6.2.9a)$$

where $\beta = \omega h$, $a_2 = h \left(\frac{3}{2} \beta^{-2} + \frac{1}{2} \beta^{-2} \cos 2\beta - \beta^{-3} \sin 2\beta \right)$,
 $c_2 = 4h\beta^{-2} (\beta^{-1} \sin \beta - \cos \beta)$.

The error, in view of (1.5.6), is given by

$$\begin{aligned} E_c(\omega) &= \int_{x_k}^{x_{k+1}} e_k(x) \, dx \\ &= \frac{h^4}{2} \int_0^2 \int_0^2 [(\xi - \tau)^2 U(\xi - \tau) + \xi(\xi - 2)(1 - \tau)^2 U(1 - \tau) \\ &\quad - \frac{1}{2} \xi(\xi - 1)(2 - \tau)^2] \, d\tau \, d\xi \sum_{k=0}^\infty f'''(x_{2k} + \tau h) \cos \omega (x_{2k} + \xi h). \end{aligned} \quad (6.2.9b)$$

Let $K(\xi, \tau)$ denote the kernel of the integrand in (6.2.9b):

$$K(\xi, \tau) = (\xi - \tau)^2 U(\xi - \tau) + \xi(\xi - 2)(1 - \tau)^2 U(1 - \tau) - \frac{1}{2} \xi(\xi - 1)(2 - \tau)^2.$$

Then $|K(\xi, \tau)| \leq 1$ in the region of integration which is the square $\{0 \leq \xi, \tau \leq 2\}$ (see [Krylov and Skoblya 1977](#), pp. 180–183). This leads to the error estimate:

$$\begin{aligned} |E_c(\omega)| &\leq \frac{h^4}{2} \int_0^2 \int_0^2 d\xi \, d\tau \sum_{k=0}^\infty |f'''(x_{2k} + \tau h)| \\ &= h^4 \int_0^2 d\tau \sum_{k=0}^\infty |f'''(x_{2k} + \tau h)| \\ &= h^4 \frac{1}{h} \int_0^\infty |f'''(x)| \, dx = h^3 V_0^\infty \{f''(x)\}. \end{aligned}$$

A less accurate estimate is

$$|E_c(\omega)| \leq h^4 \max_{0 \leq t \leq 1} \sum_{k=0}^{\infty} |f'''(x_k + ht)|. \quad (6.2.9c)$$

Similarly, for the FOURIER SINE TRANSFORM we get

$$\begin{aligned} F_s(\omega) &= \int_0^{\infty} f(x) \sin \omega x \, dx \\ &= b_2 f_0 + c_2 \sum_{k=0}^{\infty} f_{2k+1} \sin(2k+1)\beta + 2a_2 \sum_{k=0}^{\infty} f_{2k+1} \sin 2k\beta + E_s(\omega), \end{aligned} \quad (6.2.10a)$$

where $b_2 = h(\beta^{-1} - \beta^{-3} + \frac{1}{2}\beta^{-2} \sin 2\beta + \beta^{-3} \cos 2\beta)$, and the error estimate is given by

$$\begin{aligned} E_s(\omega) &= \frac{h^4}{2} \int_0^2 \int_0^2 [(\xi - \tau)^2 U(\xi - \tau) + \xi(\xi - 2)(1 - \tau)^2 U(1 - \tau) \\ &\quad - \frac{1}{2} \xi(\xi - 1)(2 - \tau)^2] \, d\tau \, d\xi \sum_{k=0}^{\infty} f'''(x_{2k} + \tau h) \sin \omega(x_{2k} + \xi h). \end{aligned} \quad (6.2.10b)$$

Hence, the bounds for $|E_s(\omega)|$ are the same as in (6.2.9c) and (6.2.10a).

For the FOURIER COMPLEX TRANSFORM, the results are

$$\begin{aligned} F(\omega) &= \int_{-\infty}^{\infty} f(t) e^{iht} \, dt \\ &= 2a_2 \sum_{k=-\infty}^{\infty} f_{2k} e^{-2ik\beta} + c_2 \sum_{k=-\infty}^{\infty} f_{2k+1} e^{-i(2k+1)\beta} + E(\omega), \end{aligned} \quad (6.2.11a)$$

$$\begin{aligned} E(\omega) &= \frac{h^4}{2} \int_0^2 \int_0^2 [(\xi - \tau)^2 U(\xi - \tau) + \xi(\xi - 2)(1 - \tau)^2 U(1 - \tau) \\ &\quad - \frac{1}{2} \xi(\xi - 1)(2 - \tau)^2] \, d\tau \, d\xi \sum_{k=-\infty}^{\infty} f'''(x_{2k} + \tau h) e^{-(x_{2k} + \tau h)\omega}, \end{aligned}$$

which yields the error bounds

$$|E(\omega)| \leq h^3 \int_{-\infty}^{\infty} |f'''(x)| \, dx = h^3 V_0^{\infty} \{f''(x)\}, \quad (6.2.11b)$$

$$|E(\omega)| \leq h^4 \max_{0 \leq \tau \leq 1} \sum_{k=-\infty}^{\infty} |f'''(x_k + \tau h)|. \quad (6.2.11c)$$

CASE 3. CUBIC INTERPOLATION WITH FOUR SINGLE POINTS. If we take 4 points x_k, x_{k+1}, x_{k+2} , and x_{k+3} , and interpolate f with respect to values at these points, then the cubic interpolation of f is given by (1.5.7). We multiply (1.5.7) by $\cos \omega x$ and integrate over the interval $[x_k, x_{k+3}]$ followed by the summation over the values of $k = 0, 3, 6, \dots$, and we obtain the following representation for the FOURIER COSINE TRANSFORM:

$$\begin{aligned} F_c(\omega) &= \int_0^\infty f(x) \cos \omega x \, dx \\ &= a_3 f_0 + \sum_{k=0}^\infty (c_3 \cos 3k\beta - d_3 \sin 3k\beta) f_{3k+1} \\ &\quad + \sum_{k=1}^\infty (c_3 \cos 3k\beta + d_3 \sin 3k\beta) f_{3k-1} + 2a_3 \sum_{k=1}^\infty f_{3k} \cos 3k\beta + E_c(\omega), \end{aligned} \quad (6.2.12a)$$

$$\begin{aligned} E_c(\omega) &= \frac{h^5}{6} \int_0^3 \int_0^3 [(\xi - \tau)^3 U(\xi - \tau) - \frac{1}{2} \xi(\xi - 2)(\xi - 3)(1 - \tau)^3 U(1 - \tau) \\ &\quad + \frac{1}{2} \xi(\xi - 1)(\xi - 3)(2 - \tau)^3 U(2 - \tau) - \frac{1}{6} \xi(\xi - 1)(\xi - 2)(3 - \tau)^3] \\ &\quad \times \sum_{k=0}^\infty f^{(4)}(x_{3k} + \tau h) \cos \omega(x_{3k} + \xi h) \, d\tau \, d\xi, \end{aligned} \quad (6.2.12b)$$

where $\beta = \omega h$, and

$$\begin{aligned} a_3 &= h \left[\frac{11}{6} \beta^{-2} - \beta^{-4} + \left(\beta^{-4} - \frac{1}{3} \beta^{-2} \right) \cos 3\beta + \beta^{-3} \sin 3\beta \right], \\ b_3 &= h \left[\beta^{-1} - 2\beta^{-3} + \left(\beta^{-4} - \frac{1}{3} \beta^{-2} \right) \sin 3\beta - \beta^{-3} \cos 3\beta \right], \\ c_3 &= h \left[3\beta^{-4} - 3\beta^{-2} + 3 \left(\frac{1}{2} \beta^{-2} - \beta^{-4} \right) \cos 3\beta - 4\beta^{-3} \sin 3\beta \right], \\ d_3 &= h \left[5\beta^{-3} + 3 \left(\frac{1}{2} \beta^{-2} - \beta^{-4} \right) \sin 3\beta + 4\beta^{-3} \cos 3\beta \right]. \end{aligned}$$

For the FOURIER SINE TRANSFORM we have:

$$\begin{aligned} F_s(\omega) &= \int_0^\infty f(x) \sin \omega x \, dx \\ &= b_3 f_0 + \sum_{k=0}^\infty (c_3 \sin 3k\beta + d_3 \cos 3k\beta) f_{3k+1} \\ &\quad + \sum_{k=1}^\infty (c_3 \sin 3k\beta - d_3 \cos 3k\beta) f_{3k-1} + 2a_3 \sum_{k=1}^\infty f_{3k} \sin 3k\beta + E_s(\omega), \end{aligned} \quad (6.2.13a)$$

$$E_s(\omega) = \frac{h^5}{6} \int_0^3 \int_0^3 [(\xi - \tau)^3 U(\xi - \tau) - \frac{1}{2} \xi(\xi - 2)(\xi - 3)(1 - \tau)^3 U(1 - \tau)$$

$$\begin{aligned}
& + \frac{1}{2} \xi(\xi-1)(\xi-3)(2-\tau)^3 U(2-\tau) - \frac{1}{6} \xi(\xi-1)(\xi-2)(3-\tau)^3] \\
& \times \sum_{k=0}^{\infty} f^{(4)}(x_{3k} + \tau h) \sin \omega(x_{3k} + \xi h) d\tau d\xi; \quad (6.2.13b)
\end{aligned}$$

and for the FOURIER COMPLEX TRANSFORM we have:

$$\begin{aligned}
F(\omega) &= \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx = (c_3 - i d_3) \sum_{k=-\infty}^{\infty} f_{3k+1} e^{-3ki\beta} \\
&+ (c_3 + i d_3) \sum_{k=-\infty}^{\infty} f_{3k-1} e^{-3ki\beta} + 2a_3 \sum_{k=-\infty}^{\infty} f_{3k} e^{-3ki\beta} + E(\omega), \quad (6.2.14a)
\end{aligned}$$

$$\begin{aligned}
E(\omega) &= \frac{h^5}{6} \int_0^3 \int_0^3 [(\xi - \tau)^3 U(\xi - \tau) - \frac{1}{2} \xi(\xi - 2)(\xi - 3)(1 - \tau)^3 U(1 - \tau) \\
&+ \frac{1}{2} \xi(\xi - 1)(\xi - 3)(2 - \tau)^3 U(2 - \tau) - \frac{1}{6} \xi(\xi - 1)(\xi - 2)(3 - \tau)^3] d\tau d\xi \\
&\times \sum_{k=0}^{\infty} f^{(4)}(x_{3k} + \tau h) e^{-i\omega(x_{3k} + \xi h)}. \quad (6.2.14b)
\end{aligned}$$

CASE 4. CUBIC INTERPOLATION WITH TWO DOUBLE POINTS. If we interpolate f over the interval $[kh, (k+1)h]$ at the points x_k , and x_{k+1} with respect to the values f_k, f_{k+1}, f'_k , and f'_{k+1} at these points by using a polynomial of degree 3, the representation of f is given by (1.5.8), and the related error by (1.5.9). After multiplying (1.5.8) by $\cos \omega x$, integrating over the interval $[kh, (k+1)h]$, and summing the results for $k = 0, 1, 2, \dots$, we find the following representation for the FOURIER COSINE TRANSFORM:

$$\begin{aligned}
E_c(\omega) &= \int_0^{\infty} f(x) \cos \omega x dx \\
&= A_1 f_0 - C_1 f'_0 + 2A_1 \sum_{k=1}^{\infty} f_k \cos k\beta - 2D_1 \sum_{k=1}^{\infty} f'_k \sin k\beta + E_c(\omega), \quad (6.2.15a)
\end{aligned}$$

where

$$\begin{aligned}
A_1 &= h (12\beta^{-4}(1 - \cos \beta) - 6\beta^{-3} \sin \beta), \\
C_1 &= h (\beta^{-2} - 6\beta^{-4} + 2\beta^{-3} \sin \beta + 6\beta^{-4} \sin \beta), \\
D_1 &= h (4\beta^{-3} - 6\beta^{-4} \sin \beta + 2\beta^{-3} \cos \beta),
\end{aligned}$$

and the error is given by

$$\begin{aligned}
E_c(\omega) &= \frac{h^5}{6} \int_0^1 \int_0^1 \{[(\xi - \tau)^3 U(\xi - \tau) + \xi^2(1 - \tau)^2[(3 - 2\xi)\tau - \xi]]\} d\tau d\xi \\
&\times \sum_{k=0}^{\infty} f^{(4)}(x_k + \tau h) \cos \omega(x_{3k} + \xi h),
\end{aligned}$$

where the integrand within the braces takes its maximum value of $1/32$, which gives the final error estimate as

$$\begin{aligned} |E_c(\omega)| &\leq \frac{h^5}{6} \cdot \frac{1}{32} \int_0^1 \int_0^1 d\tau d\xi \sum_{k=0}^{\infty} |f^{(4)}(x_k + \tau h)| \\ &= \frac{h^4}{192} \int_0^{\infty} |f^{(4)}(x)| dx = \frac{h^4}{192} V_0^{\infty} \{f'''(x)\}. \end{aligned} \quad (6.2.15b)$$

By using the mean-value theorem, this estimate is refined to

$$|E_c(\omega)| \leq \frac{h^5}{720} |f^{(4)}(x_k + \theta h)|, \quad 0 < \theta < 1. \quad (6.2.15c)$$

Similarly, for the FOURIER SINE TRANSFORM, we have

$$\begin{aligned} F_s(\omega) &= \int_0^{\infty} f(x) \sin \omega x dx \\ &= B_1 f_0 + D_1 f'_0 + 2A_1 \sum_{k=0}^{\infty} f_k \sin k\beta + 2D_1 \sum_{k=0}^{\infty} f'_k \cos k\beta + E_s(\omega), \end{aligned} \quad (6.2.16a)$$

$$\begin{aligned} E_s(\omega) &= \frac{h^5}{6} \int_0^1 \int_0^1 \{(\xi - \tau)^3 U(\xi - \tau) + \xi^2(1 - \tau)^2[(3 - 2\xi)\tau - \xi]\} d\tau d\xi \\ &\quad \times \sum_{k=0}^{\infty} f(x_k + \tau h) \sin \omega(x_k + \xi h), \end{aligned}$$

where $B_1 = h(6\beta^{-3} \cos \beta - 12\beta^{-4} \sin \beta + \beta^{-3}(6 + \beta^2))$; thus, using the mean-value theorem, we get the estimates

$$E_s(\omega) \leq \frac{h^4}{192} \int_0^{\infty} |f^{(4)}(x)| dx = \frac{h^4}{192} V_0^{\infty} \{f'''(x)\}, \quad (6.2.16b)$$

$$|E_s(\omega)| \leq \frac{h^5}{720} |f^{(4)}(x_k + \theta h)|, \quad 0 < \theta < 1. \quad (6.2.16c)$$

For the FOURIER COMPLEX TRANSFORM we have:

$$\begin{aligned} F(\omega) &= \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx \\ &= 2A_1 \sum_{k=-\infty}^{\infty} f_k e^{-ik\beta} - 2iD_1 \sum_{k=-\infty}^{\infty} f'_k e^{-ik\beta} + E(\omega), \end{aligned} \quad (6.2.17a)$$

$$\begin{aligned} E(\omega) &= \frac{h^5}{6} \int_0^1 \int_0^1 \{(\xi - \tau)^3 U(\xi - \tau) + \xi^2(1 - \tau)^2[(3 - 2\xi)\tau - \xi]\} d\tau d\xi \\ &\quad \times \sum_{k=0}^{\infty} f(x_{3k} + \tau h) e^{-i\omega(x_k + \xi h)}, \end{aligned}$$

which gives the error estimates

$$|E(\omega)| \leq \frac{h^4}{192} \int_0^\infty |f^{(4)}(x)| dx = \frac{h^4}{192} V_{-\infty}^\infty \{f'''(x)\}, \quad (6.2.17b)$$

$$|E(\omega)| \leq \frac{h^5}{720} |f^{(4)}(x_k + \theta h)|, \quad 0 < \theta < 1. \quad (6.2.17c)$$

CASE 5. CUBIC INTERPOLATION WITH THREE DOUBLE POINTS. If we interpolate f at the points x_k , x_{k+1} , and x_{k+2} with respect to the values f_k , f_{k+1} , f'_k , f'_{k+1} , f_{k+2} , and f'_{k+2} at these points, the representation of f is given by (1.5.11), and the related error by (1.5.12). After multiplying (1.5.11) by $\cos \omega x$, integrating over the interval $[x_k, x_{k+2}]$, and summing the results for $k = 0, 2, 4, \dots$, we find the following representation for the FOURIER COSINE TRANSFORM:

$$\begin{aligned} E_c(\omega) &= \int_0^\infty f(x) \cos \omega x dx \\ &= A_2 f_0 + C_2 \sum_{k=1}^\infty f_{2k+1} \cos(2k+1)\beta + 2A_2 \sum_{k=1}^\infty f'_{2k} \cos 2k\beta \\ &\quad - D_2 f'_0 - E_2 \sum_{k=0}^\infty f'_{2k+1} \sin(2k+1)\beta - 2F_2 \sum_{k=1}^\infty f'_{2k} \sin 2k\beta + E_c(\omega), \end{aligned} \quad (6.2.18a)$$

where

$$\begin{aligned} h^5 \omega^6 A_2 &= \beta (156 - 7\beta^2) \sin \beta \cos \beta + 3 (60 + 17\beta^2) \cos^2 \beta - 15 (12 - 5\beta^2), \\ h^5 \omega^6 B_2 &= \beta (\beta^4 + 8\beta^2 - 24) + \beta (7\beta^2 - 156) \cos^2 \beta + 3 (60 - 17\beta^2) \sin \beta \cos \beta, \\ h^5 \omega^6 C_2 &= 16\beta (3 - \beta^2) \sin \beta - 48\beta^2 \cos \beta, \\ h^5 \omega^6 D_2 &= 2\beta (\beta^2 - 24) \sin \beta \cos \beta + 15 (\beta^2 - 4) \cos^2 \beta + \beta^4 + 27\beta^2 + 6\beta, \\ h^5 \omega^6 E_2 &= 16\beta (\beta^2 - 15) \cos \beta + 48 (5 - 2\beta^2) \sin \beta, \\ h^5 \omega^6 F_2 &= \beta (5\beta^2 - 12) + 15 (4 - \beta^2) \sin \beta \cos \beta + 2\beta (\beta^2 - 24) \cos^2 \beta, \end{aligned}$$

and the error is given by

$$\begin{aligned} E_c(\omega) &= \frac{h^7}{6!} \int_0^2 \xi^2 (\xi - 1)^2 (\xi - 2)^2 \\ &\quad \times \sum_{k=0}^\infty f^{(4)}(x_{2k} + \theta_{2k} h) \cos \omega (x_{2k} + \xi h) d\xi. \end{aligned} \quad (6.2.18b)$$

This yields the error estimates

$$|E_c(\omega)| \leq \frac{h^7}{9450} \sum_{k=0}^\infty \max_{0 \leq \theta \leq 2} |f^{(4)}(x_k + \theta h)|. \quad (6.2.18c)$$

Similarly, for the FOURIER SINE TRANSFORM, we have

$$\begin{aligned}
 E_s(\omega) &= \int_0^\infty f(x) \sin \omega x \, dx \\
 &= B_2 f_0 + C_2 \sum_{k=1}^\infty f_{2k+1} \sin(2k+1)\beta + 2A_2 \sum_{k=1}^\infty f'_{2k} \sin 2k\beta \\
 &\quad + F_2 f'_0 + E_2 \sum_{k=0}^\infty f'_{2k+1} \cos(2k+1)\beta + 2F_2 \sum_{k=1}^\infty f'_{2k} \cos 2k\beta + E_c(\omega), \\
 E_c(\omega) &= \frac{h^7}{6!} \int_0^2 \xi^2 (\xi-1)^2 (\xi-2)^2 \\
 &\quad \times \sum_{k=0}^\infty f^{(4)}(x_{2k} + \theta_{2k}h) \sin \omega (x_{2k} + \xi h) \, d\xi,
 \end{aligned} \tag{6.2.19a}$$

which gives the error estimate

$$|E_s(\omega)| \leq \frac{h^7}{9450} \sum_{k=0}^\infty \max_{0 \leq \theta \leq 2} |f^{(4)}(x_{2k} + \theta h)|. \tag{6.2.19b}$$

For the FOURIER COMPLEX TRANSFORM we have

$$\begin{aligned}
 E(\omega) &= \int_{-\infty}^\infty f(x) e^{-i\omega x} \, dx \\
 &= 2A_2 \sum_{k=-\infty}^\infty f_{2k} e^{-2ik\beta} + C_2 \sum_{k=-\infty}^\infty f'_{2k+1} e^{-i(2k+1)\beta} \\
 &\quad - 2iF_2 \sum_{k=-\infty}^\infty f'_{2k} e^{-2ik\beta} - iE_2 \sum_{k=-\infty}^\infty f'_{2k+1} e^{-i(2k+1)\beta} + E(\omega),
 \end{aligned} \tag{6.2.20a}$$

$$|E(\omega)| \leq \frac{h^7}{9450} \sum_{k=-\infty}^\infty \max_{0 \leq \theta \leq 2} |f^{(4)}(x_{2k} + \theta h)|. \tag{6.2.20b}$$

6.2.2. Hurwitz-Zweifel's Method. Hurwitz and Zweifel (1956) consider integrals of the form

$$S(x) = \int_0^\infty f(\omega) \sin(x\omega) \, d\omega, \tag{6.2.21a}$$

$$C(x) = \int_0^\infty g(\omega) \cos(x\omega) \, d\omega, \tag{6.2.21b}$$

which appear in applied mathematical problems and need to be computed. Assuming that the functions f and g are such that $f(-x) = -f(x)$ and $g(-x) = g(x)$, they

use the Gaussian-Chebyshev quadrature (§3.2.7) on the interval $[-\frac{1}{2}, \frac{1}{2}]$ to derive an approximation formula by performing the sum over half cycles and using standard techniques for accelerating the convergence of the sums of an oscillating series. First, the range is extended to $-\infty \leq x \leq \infty$ by setting $y = x\omega/\pi - \frac{1}{2}$ in (6.2.21a) and $u = x\omega/\pi$ in (6.2.21b), and extending the definition of f and g to $f(-x) = -f(x)$ and $g(-x) = g(x)$. Then the integrals (6.2.21a,b) become

$$S(x) = \frac{\pi}{2x} \int_{-1/2}^{1/2} \sigma(y, x) \cos \pi y dy, \quad (6.2.22a)$$

$$C(x) = \frac{\pi}{2x} \int_{-1/2}^{1/2} \gamma(u, x) \cos \pi u du, \quad (6.2.22b)$$

where

$$\sigma(y, x) = \sum_{n=-\infty}^{\infty} (-1)^n f\left(\frac{\pi}{x} \left(y + n + \frac{1}{2}\right)\right),$$

$$\gamma(u, x) = \sum_{n=-\infty}^{\infty} (-1)^n g\left(\frac{\pi}{x} (u + n)\right).$$

The function $\sigma(y, x)$ has the following properties: (i) $\sigma(y, x) = \sigma(-y, x)$; (ii) $\sigma(\frac{1}{2}, x) = \sigma(-\frac{1}{2}, x) = 0$; (iii) $\sigma(y + n, x) = (-1)^n \sigma(y, x)$; and (iv) σ is regular in $-\frac{1}{2} \leq y \leq \frac{1}{2}$ if $f(x)$ is regular in $-\infty \leq x \leq \infty$. Because of these properties, σ can be expanded as a Fourier series of the form

$$\sigma(y, x) = \sum_{n=0}^{\infty} a_n(x) \cos(2n+1)\pi y = \cos \pi y \sum_{n=0}^{\infty} \alpha_n \cos^{2n} \pi y, \quad (6.2.23)$$

using the fact that $\cos n\theta$ is a polynomial in $\cos \theta$. A similar expression can be written for $\gamma(u, x)$. If we substitute (6.2.23) into (6.2.22a), we obtain

$$S(x) = \frac{\pi}{2x} \int_{-1/2}^{1/2} \cos^2 \pi y \sum_{n=0}^{\infty} \alpha_n(x) \cos^{2n} \pi y.$$

Then a set of polynomials in $\cos^2 \pi y$ orthogonal on the interval $(-1/2, 1/2)$ with the weight function $\cos^2 \pi y$ is found. Let $G_n(\cos \pi y)$ represent these polynomials with the orthogonality relation

$$\int_{-1/2}^{1/2} \cos^2 \pi y G_n(\cos \pi y) G_m(\cos \pi y) dy = 0 \quad \text{for } n \neq m.$$

Since the polynomials $G_n(\cos \pi y)$ are related to the Chebyshev polynomials of the first kind $T_n(x)$ by $G_n(\cos \pi y) = \cos(\pi y)^{-1} T_{2n+1}(\cos \pi y) = \cos(\pi y)^{-1} \cos(2n+1)\pi y$, we obtain the $2N$ -point Gauss-Chebyshev quadrature formula

$$\int_{-1/2}^{1/2} \sigma(y, x) \cos \pi y dy = \sum_{j=1}^N \frac{2\lambda_j^{(N)}}{\cos \pi y_j^{(N)}} \sigma\left(y_j^{(N)}, x\right), \quad (6.2.24)$$

where the nodes $y_j^{(N)}$, which are the zeros of $G_N(\cos \pi y)$, are given by

$$y_j^{(N)} = \frac{2j-1}{2(2N+1)}, \quad j = 1, 2, \dots, N,$$

and the weights $\lambda_j^{(N)}$ are the so-called Christoffel numbers (see §5.1.1). These nodes and weights for the 2- and 4-point formulas are: (i) for the 2-point formula ($N = 1$): $y_1 = 1/6$, $\cos \pi y_1 = \sqrt{3}/2$, $\lambda_1 = 1/4$; and (ii) for the 4-point formula ($N = 2$): $y_1 = 3/10$, $y_2 = 1/10$, $\cos \pi y_1 = 0.5877852$, $\cos \pi y_2 = 0.9510565$, $\lambda_1 = 0.06909832$, $\lambda_2 = 0.18090169$. It is found that the 2-point formula gives sufficient accuracy. Formula (6.2.24) is exact only if $\frac{\sigma(y, x)}{\cos \pi y}$ is independent of y . A special case of (6.2.24) is $\int_{-1/2}^{1/2} \sigma(y, x) \cos \pi y dy = \frac{1}{2} \sigma(0, x)$.

Since

$$\int_{-1/2}^{1/2} \cos^{2k} y dy = \frac{1}{\sqrt{\pi}} \frac{\Gamma(k + \frac{1}{2})}{\Gamma(k + 1)},$$

the weights $\lambda_j^{(N)}$ are the solutions of the N simultaneous equations

$$\frac{\Gamma(k + \frac{1}{2})}{\Gamma(k + 1)} = 2 \sum_{j=1}^N \cos^{2k-2} \left(\frac{[2j-1]\pi}{2[2N+1]} \lambda_j^{(N)} \right), \quad k = 1, 2, \dots, N.$$

These weights are already calculated in §5.1.1.

EXAMPLE 6.2.1. Consider $g(x) = (1 + L^2 x^2)^{-1}$, where L is a constant. Then the integral (6.2.21b) is evaluated analytically to give $C(x) = \frac{\pi}{2L} e^{-\hat{x}}$, where $\hat{x} = x/L$, and the $2N$ -point quadrature formula yields

$$C(x) = \frac{\pi}{2x} \sum_{j=1}^N \frac{2\lambda_j^{(N)}}{\cos \pi y_j^{(N)}} \gamma(y_j^{(N)}, x), \quad (6.2.25)$$

where

$$\begin{aligned} \gamma(y_j^{(N)}, x) &= \sum_{n=-\infty}^{\infty} (-1)^n \frac{x^2}{x^2 + L^2 \pi^2 (y_j^{(N)} + n)^2} \\ &= \frac{\hat{x} \sinh \hat{x} \cos \pi y_j^{(N)}}{\sin^2 \pi y_j^{(N)} \cosh^2 \hat{x} + \cos^2 \pi y_j^{(N)} \sinh^2 \hat{x}}, \end{aligned} \quad (6.2.26a)$$

$$\frac{\gamma(y_j^{(N)}, x)}{\cos \pi y_j^{(N)}} = 2 \hat{x} \{e^{-\hat{x}} - e^{-3\hat{x}}\} [1 + (4 \cos^2 \pi y_j^{(N)} - 2) e^{-2\hat{x}} + \dots]. \quad (6.2.26b)$$

Thus, (6.2.26b) implies that (6.2.23) converges rapidly for large x , and (6.2.25) and (6.2.26b) imply that in the limit $C(x) = \frac{\pi}{2L} e^{-\hat{x}} + O(e^{-3\hat{x}})$ for large x , independent of N , so that even a 1-point formula is useful. But as x decreases, one should go to larger values of N . ■

A drawback of this method is that the value of ω at which $f(\omega)$ or $g(\omega)$ is to be computed depends on the value of the parameter x . Thus, the method is useful when the results are needed only for a few values of x .

To facilitate computation, define

$$S(x) = \frac{\pi}{x} \sum_{n=0}^{\infty} S_n(x), \quad C(x) = \frac{\pi}{x} \left[\frac{1}{2} C_0(x) + \sum_{n=0}^{\infty} C_n(x) \right],$$

where

$$\begin{aligned} S_n(x) &= (-1)^n \int_{-1/2}^{1/2} f\left(\frac{\pi}{x} \left(y + n + \frac{1}{2}\right)\right) \cos \pi y \, dy \\ &= (-1)^n \sum_{j=0}^N \frac{\lambda_j^{(N)}}{\cos \pi y_j^{(N)}} \left\{ f\left(\frac{\pi}{x} \left(y_j^{(N)} + n + \frac{1}{2}\right)\right) \right. \\ &\quad \left. + f\left(\frac{\pi}{x} \left(-y_j^{(N)} + n + \frac{1}{2}\right)\right) \right\}, \\ C_n(x) &= (-1)^n \int_{-1/2}^{1/2} g\left(\frac{\pi}{x} (u + n)\right) \cos \pi u \, du \\ &= (-1)^n \sum_{j=0}^N \frac{\lambda_j^{(N)}}{\cos \pi u_j^{(N)}} \left\{ g\left(\frac{\pi}{x} \left(y_j^{(N)} + n\right)\right) + g\left(\frac{\pi}{x} \left(-y_j^{(N)} + n\right)\right) \right\}. \end{aligned}$$

AVERAGING TECHNIQUE. As suggested by M. Ray in Hurwitz and Steifel (1956), form the sequence of partial sums $\beta_n = \sum_{k=0}^n S_k(x)$, so that $S(x) = \frac{\pi}{x} \lim_{n \rightarrow \infty} \beta_n$. Then find the limit of the sequence $\{\beta_n\}$ by the ‘averaging technique’ which is achieved by defining

$$\begin{aligned} a_1^{(n)} &= \frac{1}{2} (\beta_n + \beta_{n+1}), \\ a_2^{(n)} &= \frac{1}{2} (a_1^{(n)} + a_1^{(n+1)}), \\ &\dots \quad \dots \quad \dots \quad \dots \quad \dots \\ a_k^{(n)} &= \frac{1}{2} (a_{k-1}^{(n)} + a_{k-1}^{(n+1)}), \end{aligned}$$

for which see Knopp (1928, §114, p. 244). Then $\lim_{n \rightarrow \infty} \beta_n = \lim_{k \rightarrow \infty} a_k$. The sequence a_k generally converges more rapidly than the sequence β_n .

Table 6.2.1.

n	f	S_n	β_n	$a_1^{(n)}$
10	0.2776371	0.1388186	0.0668927	2.6191(−3)
11	0.2570943	−0.1285472	−0.0616545	−1.8693(−3)
12	0.2391407	0.1195704	0.0579159	2.0741(−3)
13	0.2233671	−0.1116836	−0.0537677	−1.4098(−3)
14	0.2094314	0.1047157	0.0509480	1.6853(−3)
15	0.1970509	−0.0985254	−0.0475774	−1.0791(−3)
16	0.1859931	0.0929966	0.0454192	

Table 6.2.2.

n	$a_1^{(n)}$	$a_2^{(n)}$	$a_3^{(n)}$	$a_4^{(n)}$	$a_5^{(n)}$
10	2.6191(−3)	3.749(−4)	2.386(−4)	2.271(−4)	2.270(−4)
11	−1.8693(−3)	1.024(−4)	2.173(−4)	2.270(−4)	
12	2.0741(−3)	3.322(−4)	2.350(−4)		
13	−1.4098(−3)	1.378(−4)	2.204(−4)		
14	1.6853(−3)	3.031(−4)			
15	−1.0791(−3)				

EXAMPLE 6.2.2. Compute $S(x) = \int_0^\infty \frac{\omega}{1 + \omega^2} \sin \omega x \, d\omega$, which has the exact value $\frac{\pi}{2} e^{-x}$. Table 6.2.1 gives the values of $f\left(\frac{\pi}{x} \left(y + n + \frac{1}{2}\right)\right)$ in column 2, of $S_n = (-1)^n \lambda_1 f\left(\frac{\pi}{x} \left(y + n + \frac{1}{2}\right)\right)$ in column 3, of β_n in column 4, and $a_1^{(n)}$ in column 5 for $n = 10(1)16$. The values of $a_1^{(n)}$ are then interpolated in Table 6.2.2 to obtain the limit of the sequence $a_1^{(n)}$, thus implying that we can take $S(x) \approx \frac{\pi}{x} a_5^{(n)}$. Then we obtain the computed value of $S(x) \approx 7.131 \times 10^{-5}$ for $x = 10$, which compares very well to the exact value 7.1314×10^{-5} , where the error introduced by the quadrature rule is of the order $e^{-2x} = e^{-20} = 2 \times 10^{-9}$. ■

6.3. Interpolatory Rules by Rational Functions

The use of interpolating polynomials is not always computationally convenient. In this method we need to partition the interval of integration $[0, \infty)$ or $(-\infty, \infty)$ into an infinite number of subintervals of finite length. This number depends on the rate of decrease of the function f as $|x| \rightarrow \infty$. The faster this rate is, the less the number

of the subintervals is. We will combine the Fourier cosine and sine transforms into a single integral with the exponential function $e^{i\omega x}$. Thus, we consider

$$F_e(\omega) = \int_0^\infty f(x) e^{i\omega x} dx, \quad (6.3.1)$$

where for real-valued f the real and imaginary parts of (6.3.1) represent the Fourier cosine and sine transform, respectively. If the function f is such that $f(x) = F(x)(1+x)^{-s}$, $s > 1$, and $F \in C[0, \infty]$, then, as in §1.5, we write $f(x) = (1+x)^{-s} F(x) = (1+x)^{-s} [P_n(x) + e_n(x)]$, where $P_n(x)$ has the representation (1.5.13). This gives the representation for $F(\omega)$ as

$$\begin{aligned} F(\omega) &= \int_0^\infty e^{i\omega x} (1+x)^{-s} [P_n(x) + e_n(x)] dx \\ &= \sum_{k=0}^n F(x_k) \sum_{m=0}^n A_{km} \int_0^\infty e^{i\omega x} (1+x)^{-n+m-s} dx + R_n(\omega), \end{aligned} \quad (6.3.2)$$

$$R_n(\omega) = \int_0^\infty e^{i\omega x} (1+x)^{-s} e_n(x) dx, \quad (6.3.3)$$

where $A_{km} = c_m^{(k)} \frac{(1+x_k)^n}{\pi'(x_k)}$ depend only on the points x_k and not on s or F . The integrals $\int_0^\infty e^{i\omega x} (1+x)^{-n+m-s} dx$ depend only on ω and s , which depends on how fast $f(x)$ decreases as x increases without bound. The rules for computing these integrals are given below in §6.3.2. An estimate for the remainder (6.3.3) in terms of the interpolation error $e_n(x)$ is given by

$$|R_n(\omega)| \leq \int_0^\infty \frac{|e_n(x)|}{(1+x)^s} dx. \quad (6.3.4)$$

If, for all sufficiently large values of n , the interpolation error $e_n(x)$ is such that $|e_n(x)| \leq M < \infty$ for $0 \leq x < \infty$, then the remainder $R_n(\omega)$ tends to zero uniformly with respect to ω on the axis $-\infty < \omega < \infty$ as $n \rightarrow \infty$ (Krylov and Skoblya, 1977, pp. 213–214).

6.3.1. Equally Spaced Interpolation Points. Let the points x_k be equally spaced such that $x_k = kh$, $k = 0, 1, \dots$, and $h > 0$. Then $\pi_{n+1}(x) = x(x-h) \dots (x-nh)$, and the coefficients $c_m^{(k)}$ in A_{km} are computed from

$$\begin{aligned} \frac{\pi_{n+1}(x)}{x - x_k} &= x(x-h) \dots [x - (k-1)h][x - (k+1)h] \dots (x-nh) \\ &= \sum_{m=0}^n c_m^{(k)} (1+x)^m, \quad k = 0, 1, \dots, n, \end{aligned} \quad (6.3.5)$$

In the case of uniform convergence, we have

$$\begin{aligned}\pi'(x_k) &= kh(k-1)h \dots h(-h)(-2h) \dots (-1)(n-k)h \\ &= h^n(-1)^{n-k} k!(n-k)!,\end{aligned}$$

which yields

$$A_{km} = \frac{c_m^{(k)}(1+kh)^n}{(-1)^{n-k} h^n k!(n-k)!}. \quad (6.3.6)$$

While computing the tables for the values of A_{km} , we assume $h = 1$, since any other value of h leads to 1 through linear transformation $x = hx'$. Note that the tables of values of A_{km} ($k, m = 0, 1, \dots, n$) for $n = 1(1)15$ and $h = 1$ to 10S are available in Krylov and Kruglikova 1968).

For equally spaced interpolation points the representation (6.3.2) becomes

$$\begin{aligned}F(\omega) &= \int_0^\infty e^{i\omega x} \frac{F(x)}{(1+x)^s} dx \\ &= \sum_{k=0}^n F(kh) \sum_{m=0}^n A_{km} \int_0^\infty e^{i\omega x} (1+x)^{-n+m-s} dx + R_n(\omega).\end{aligned} \quad (6.3.7)$$

6.3.2. Computation of the Integrals $\int_0^\infty e^{i\omega x} (1+x)^{-m-\nu} dx \equiv I_{m+\nu}$, where $m \geq 0$ is an integer and $0 \leq \nu < 1$. We use integration by parts:

$$\begin{aligned}I_{m+\nu} &= \int_0^\infty e^{i\omega x} (1+x)^{-m-\nu} dx \\ &= -\frac{e^{i\omega x}}{(m-1+\nu)(1+x)^{m-1+\nu}} \Big|_0^\infty + \frac{i\omega}{m-1+\nu} \int_0^\infty \frac{e^{i\omega x} dx}{(1+x)^{m-1+\nu}} \\ &= \frac{1}{m-1+\nu} + \frac{i\omega}{m-1+\nu} \int_0^\infty \frac{e^{i\omega x} dx}{(1+x)^{m-1+\nu}},\end{aligned}$$

which gives the recurrence formula

$$I_{m+\nu} = \frac{1}{m-1+\nu} + \frac{i\omega}{m-1+\nu} I_{m+\nu-1}. \quad (6.3.8)$$

Now, we will consider the integral I_ν for $0 < \nu \leq 1$. If we set $1+x = t$, we get $I_\nu = e^{-i\omega} \int_1^\infty e^{i\omega t} t^{-\nu} dt$. For $\nu = 1$ we have

$$I_1 = e^{-i\omega} \left[\int_1^\infty \frac{\cos \omega t}{t} dt + t \int_1^\infty \frac{\sin \omega t}{t} dt = -e^{-i\omega} [\text{Ci}(\omega) + t \text{Si}(\omega)], \quad (6.3.9) \right]$$

where $\text{Ci}(\omega)$ and $\text{Si}(\omega)$ are the cosine and sine integrals, respectively. For $0 < \nu < 1$, we obtain

$$\begin{aligned}\int_1^\infty e^{i\omega t} \frac{dt}{t^\nu} &= \int_0^\infty e^{i\omega t} \frac{dt}{t^\nu} - \int_0^1 e^{i\omega t} \frac{dt}{t^\nu}, \\ \int_0^\infty e^{i\omega t} \frac{dt}{t^\nu} &= \omega^{\nu-1} \Gamma(1-\nu) e^{i\pi(1-\nu)/2}, \quad \omega > 0, \\ \int_0^1 e^{i\omega t} \frac{dt}{t^\nu} &= \sum_{k=0}^\infty \frac{(i\omega)^k}{k!} \int_0^1 t^{k-\nu} dt = \sum_{k=0}^\infty \frac{(i\omega)^k}{(k+1-\nu) k!}.\end{aligned}$$

Thus,

$$\begin{aligned}I_\nu &= \int_0^\infty e^{i\omega t} \frac{dt}{(1+x)^\nu} = \omega^{\nu-1} \Gamma(1-\nu) e^{i(\pi(1-\nu)/2-\omega)} \\ &\quad + e^{-i\omega} \sum_{k=0}^\infty \frac{(i\omega)^k}{(k+1-\nu) k!}.\end{aligned}\tag{6.3.10}$$

6.3.3. High-Precision Formulas. If $f(x) = (1+x)^{-s} F(x)$, $s > 1$, then

$$F_c(\omega) = \int_0^\infty f(x) \cos \omega x dx = \int_0^\infty \frac{\cos \omega x}{(1+x)^s} F(x) dx.$$

With the weight function $w(x) = (1+x)^{-s} \cos \omega x$, we construct a quadrature formula of the form

$$\int_0^\infty \frac{\cos \omega x}{(1+x)^s} F(x) dx \approx \sum_{k=1}^n A_k F(x_k).\tag{6.3.11}$$

There are $2n$ parameters A_k and x_k , and we choose them such that (6.3.11) becomes exact when $F(x)$ is a polynomial of degree $2n-1$ in $(1+x)^{-1}$, which implies that for $2n$ simple fractions $(1+x)^{-j}$, $j = 0, 1, \dots, 2n-1$, we must have

$$\int_0^\infty (1+x)^{-s-j} \cos \omega x dx = \sum_{k=1}^n A_k (1+x_k)^{-j}.\tag{6.3.12}$$

These equations form a system of $2n$ equations, which is linear in A_k and nonlinear in x_k , and determines the parameters A_k and x_k . The defect with this approach is that even for small values of n the points x_k are found to lie outside the interval $[0, \infty)$. This is because of the varying sign property of the weight function $w(x)$. Thus, to avoid this defect, we must make the weight function to have a constant sign. This is done by writing

$$\int_0^\infty \cos \omega x f(x) dx = \int_0^\infty (1 + \cos \omega x) f(x) dx - \int_0^\infty f(x) dx \equiv I_c^1 - I_c^2.$$

If we set $\omega x = u$, $\omega \geq 1$ in I_c^1 , then

$$I_c^1 = \int_0^\infty (1 + \cos u) \frac{1}{\omega} f\left(\frac{u}{\omega}\right) du = \int_0^\infty (1 + \cos x) X(x) dx,$$

where $X(x) = \frac{1}{\omega} f\left(\frac{u}{a}\right)$. Suppose that $X(x)$ is represented as $X(x) = \frac{F(x)}{(1+x)^s}$, $s > 1$. Then

$$I_c^1 = \int_0^\infty (1 + \cos x) X(x) dx = \int_0^\infty \frac{1 + \cos x}{(1+x)^s} F(x) dx, \quad (6.3.13)$$

which has the positive weight $1 + \cos x$ or $(1 + \cos x)(1+x)^{-s}$. Next, the integral I_c^2 is reduced an integral with the Jacobi weight function with parameters 0 and $s-2$, by setting $x = (1-t)/(1+t)$:

$$I_c^2 = \int_0^\infty f(x) dx = \int_0^\infty \frac{F(x)}{(1+x)^s} dx = 2^{1-s} \int_{-1}^1 F\left(\frac{1-t}{1+t}\right) (1+t)^{s-2} dt, \quad (6.3.14)$$

which can be easily computed.

Also, since $I_c^1 = \int_0^\infty (1 + \cos x) X(x) dx \approx \sum_{k=1}^n A_k X(x_k)$, we choose the parameters A_k and x_k such that the this rule is exact for functions $(1+x)^{-s-j}$, $s > 0$, $j = 0, 1, \dots, 2n-1$, or for all functions of the form $(1+x)^{-s} \sum_{k=0}^{2n-1} c_k (1+x)^{-k} = (1+x)^{-s-2n+1} P_{2n-1}(x)$, where $P_{2n-1} \in \mathcal{P}_{2n-1}$. This gives

$$\int_0^\infty \frac{1 + \cos x}{(1+x)^{2n-1+s}} P_{2n-1}(x) dx = \sum_{k=1}^n B_k P_{2n-1}(x_k), \quad (6.3.15)$$

$$B_k = \frac{A_k}{(1+x_k)^{2n-1+s}}.$$

Thus, the problem of computing the parameters B_k and x_k on the interval $[0, \infty)$ reduces to that of constructing a quadrature rule of highest precision with the positive weight function $(1 + \cos x)(1+x)^{-2n+1-s}$. This leads to the product quadrature formula for the integral I_c^1 , which is obtained by setting $1/(1+x) = t$, $x = 1/t - 1$, $0 < t \leq 1$ in (6.3.13); thus,

$$I_c^1 = \int_0^1 (1 + \cos x) t^{s-2} F^*(t) dt \approx \sum_{j=1}^n A_j^* F^*(t_k) = Q_n^*(F^*), \quad (6.3.16)$$

where $F^*(t) = F(1/t - 1) = F(x)$, and $t_k = 1/(1+x_k)$. This formula is exact if $F^*(t) = P_{2n-1}(t)$.

6.4. Trigonometric Integrals

We discuss trigonometric integrals of the form $\int_a^b f(x) e^{i\beta x} dx$, β real (or complex), which involve a special case of the Fourier coefficients when a period of the trigonometric functions coincides with the interval of integration, i.e., when $\beta = 2\pi n/(b-a)$, where n is an integer. The trigonometric integrals are special cases of the integral $\int_a^b f(x) e^{\beta x} dx$. We will study the following two cases: (i) $f(x)$ is a real function of a real variable x , and (ii) $f(x)$ is well behaved on the interval $[a, b]$ and determine quadrature rules which involve nodes on the real axis. Note that in this section we do not consider Fourier transforms of the form $\int_a^\infty f(x) e^{i\beta x} dx$ or $\int_{-\infty}^\infty f(x) e^{i\beta x} dx$.

We use the following notation and definitions which resemble the ones used in Fourier theory: A *periodic extension* $\hat{f}(x)$ of $f(x)$ with respect to the interval of integration $[0, 1]$ is defined by

$$\begin{cases} \hat{f}(x) = f(x), & x \in [0, 1], \\ \hat{f}(1) = \hat{f}(0) = \frac{1}{2} [f(1) + f(0)], \\ \hat{f}(x+1) = \hat{f}(x) & \text{for all } x. \end{cases}$$

Thus, $\hat{f}(x)$ has some kind of discontinuity at integer values of x when f is well behaved. Next, we will write

$$C^{(k)} f = \int_0^1 f(x) \cos 2\pi kx \, dx, \quad S^{(k)} f = \int_0^1 f(x) \sin 2\pi kx \, dx, \quad (6.4.1)$$

which are known as Fourier coefficients. Then the Fourier series for $\hat{f}(x)$ can be expressed as

$$\begin{aligned} \hat{f}(x) &= I_0^1(f) + 2 \sum_{k=1}^{\infty} \left\{ C^{(k)} f \cos 2\pi kx + S^{(k)} f \sin 2\pi kx \right\} \\ &= \sum_{k=-\infty}^{\infty} \left(C^{(k)} f + i S^{(k)} f \right) e^{-2\pi i kx} dx. \end{aligned} \quad (6.4.2)$$

Some useful formulas are: (i) The Fourier coefficient has the asymptotic expansion

$$C^{(k)} f = \frac{f'(1) - f'(0)}{(2\pi k)^2} - \frac{f^{(3)}(1) - f^{(3)}(0)}{(2\pi k)^4} + \dots, \quad (6.4.3)$$

which usually diverges but may converge to some value other than $C^{(k)} f$. If $f'(1) \neq f'(0)$, we must use good numerical approximations to $f'(1)$ and $f'(0)$ for very large

k . Also, if $f^{(s)}(1) = f^{(l)}(0)$ for $l = 0, 1, \dots, n-2$, then $C^{(k)}f + iS^{(k)}f = O(k^{-n+1})$, and the Fourier series (6.4.2) converges faster than the usual case, and we say that the function $\hat{f} \in C^{(n-1)}(-\infty, \infty)$, which implies that f is ‘nearly’ periodic. In the case when f is periodic, the functions $f(x)$ and $f(x-1)$ coincide and $f^{(l)}(1) = f^{(0)}(1) = 0$ for all l . We denote the m -panel trapezoidal rule on the interval $[0, 1]$ by

$$\begin{aligned} T^{[m,1]}(f) &= \frac{1}{m} \sum_{j=0}^m{}'' f(j/m) \\ &\equiv \frac{1}{m} \left[\frac{1}{2} f(0) + \sum_{j=1}^{m-1} f(j/m) + \frac{1}{2} f(1) \right], \end{aligned} \quad (6.4.4)$$

and the Poisson summation formula is

$$T^{[m,1]}f = I_0^1(f) + 2 \sum_{k=1}^{\infty} C^{(km)}f. \quad (6.4.5)$$

6.4.1. Basic Interpolatory Formulas. Consider the interpolation function $G(x)$ such that

$$\text{either} \quad G(j/m) = g(j/m), \quad j = 0, 1, \dots, m, \quad (6.4.6a)$$

$$\text{or} \quad G(j/m) = \hat{g}(j/m), \quad j = 0, 1, \dots, m, \quad (6.4.6b)$$

and approximate functionals involving $g(x)$ by exact evaluation of the same functional involving $G(x)$. There are three different types of interpolation functions:

TYPE 1. TRIGONOMETRIC INTERPOLATION. Let $G(x) \in \mathcal{P}_{m/2-1}$ with an additional cosine term:

$$G(x) = 2 \sum_{k=0}^{m/2}{}'' \mu_k \cos 2\pi kx + \sum_{k=1}^{m/2}{}'' \nu_k \sin 2\pi kx. \quad (6.4.7)$$

The function $G(x)$ of this form that satisfies (6.4.6b) has coefficients

$$\mu_k = T^{[m,1]}(g(x) \cos 2\pi kx), \quad (6.4.8)$$

and the Fourier coefficients of (6.4.7) are

$$C^{(k)}g = C^{(k)}G = \begin{cases} \mu_k, & k = 0, 1, \dots, m/2 - 1, \\ \frac{1}{2} \mu_{m/2}, & k = m/2, \\ 0, & k > m/2. \end{cases} \quad (6.4.9)$$

TYPE 2. PERIODIC-TYPE INTERPOLATION. If we choose linear splines $G_{11}(x)$ satisfying (6.4.6b), we obtain the Fourier coefficients

$$C^{(k)}g = C^{(k)}G_{11} = \tau(k/m)T^{[m,1]}(g(x) \cos 2\pi kx), \quad (6.4.10)$$

$$\tau(k/m) = \left(\frac{\sin \pi km}{\pi km} \right)^2,$$

where $\tau(z)$ is known as an *attenuation factor*. In the case of higher order periodic splines the Fourier coefficients are of the same form as (6.4.10) with different attenuation factors. The results are the same for interpolations is the ‘periodic type’; For a periodic function, $G(x)$ is the same function of $\hat{g}(j/m)$ as $G(x + 1/m)$ is of $\hat{g}((j + 1)/m)$ for $0, \pm 1, \pm 2, \dots$

TYPE 3. LOCAL PERIODIC INTERPOLATION. The interpolation function is a piecewise continuous interpolating polynomial of degree d , where m/d is an integer. It has m/d independent interpolating polynomials. The resulting formulas are known as *Filon-Luke formulas* (§6.6.7; also see §3.7 for Filon’s formula). However, for $d = 1$, the interpolating function is the linear spline and the Fourier coefficient is given by (6.4.10). This rule is sometimes known as the *Filon Trapezoidal rule*.

6.4.2. Euler Expansion. The Euler expansion of $f(x) \in \mathcal{P}_{n-1}$ is

$$f(x) = H_{n-1} + g_n(x), \quad (6.4.11)$$

$$H_{n-1}(x) = \sum_{q=1}^{n-1} \lambda_q \frac{B_q(x)}{q!} \quad (6.4.12,)$$

$$\lambda_q = f^{(q-1)}(1) - f^{(q-1)}(0), \quad (6.4.13)$$

where $B_q(x)$ is the Bernoulli polynomial of degree q , and $g_n(x)$ is not periodic, but it has a rapidly convergent Fourier series. This expansion is generally divergent, but if operated on both sides with the trapezoidal rule operators, we obtain the Euler-Maclaurin asymptotic expansion (2.2.8) which is used as a theoretical basis for the Romberg integration. An useful property of $g_n(x)$ is

$$g_n^{(l)}(1) - g_n^{(l)}(0) = 0, \quad l = 0, 1, \dots, n-2.$$

From (6.4.11) we obtain the formula

$$\int_0^1 f(x) e^{\beta x} dx = \int_0^1 H_{n-1} e^{\beta x} dx + \int_0^1 g_n(x) e^{\beta x} dx. \quad (6.4.14)$$

But since $\beta = 2i\pi l$ in the case of the Fourier coefficients, and since

$$\int_0^1 \frac{B_q(x)}{q!} e^{2i\pi l x} dx = -\left(\frac{1}{2i\pi l} \right)^q, \quad q, l > 0,$$

we have

$$\int_0^1 f(x) e^{2i\pi lx} dx = \sum_{q=1}^{n-1} \frac{-\lambda_q}{(2\pi i q)^l} + \int_0^1 g_n(x) e^{2i\pi lx} dx, \quad (6.4.15)$$

the real part of which is (6.4.3). Using the m -point trapezoidal rule, the above integral (6.4.15) yields

$$\begin{aligned} C^{(l)} f + i S^{(l)} f &= \mu_0 \\ &= \begin{cases} \mu_l + i \nu_l - \sum_{q=1}^{n-1} \frac{\lambda_q}{(2\pi i l)^q}, & 1 \leq l < m/2, \\ \frac{1}{2} \mu_{m/2} - \sum_{q=1}^{n-1} \frac{\lambda_q}{(\pi i m)^q}, & l = m/2, \\ - \sum_{q=1}^{n-1} \frac{\lambda_q}{(2\pi i l)^q}, & l > m/2, \end{cases} \end{aligned} \quad (6.4.16)$$

where

$$\mu_l + i \nu_l = T^{[m,1]}(g_n(x) e^{2i\pi lx}).$$

Formula (6.4.16) gives the exact Fourier coefficients of $F(x) = H_{n-1}(x) + G_n^{(m)}(x)$, where $G_n^{(m)}(x)$ is the trigonometric interpolation function of $g_n(x)$ defined by (6.4.7). Note that the first relation in (6.4.16) is known as the *Euler-Maclaurin quadratic rule*. Formula (6.4.16) is exact for $f \in \mathcal{P}_{n-1}$ for any value of m . If $f(x)$ is a trigonometric polynomial of degree $m/2 - 1$ or less, we have $H_{n-1}(x) = 0$, $G_n^{(m)}(x) = g_n(x) = f(x)$, and formulas (6.4.16) are exact. The theory is redundant whenever $\hat{f}(x) \in C^\infty[-\infty, \infty]$ and $H_{n-1}(x) = 0$. The function $H_{n-1}(x)$ in formulas (6.4.16) may be replaced by any polynomial function, but the final values of μ_l and ν_l for l near $m/2$ provide a criterion for accuracy in all approximations.

Let $\phi_d(x; f; t_0, t_1, \dots, t_d)$ or $\phi_d(x; f; \mathbf{t})$ (or simply $\phi(x)$ if there is no confusion) denote the polynomial of degree d which interpolates $f(x)$ at $x = t_0, t_1, \dots, t_d$. Set

$$\mathbf{f} = [f(t_0), f(t_1), \dots, f(t_d)]^T,$$

and let

$$\mathbf{a} = \left[\phi(0), \phi'(0), \frac{\phi''(0)}{2!}, \dots, \frac{\phi^{(d)}(0)}{d!} \right]$$

denote the Taylor's coefficients of the interpolating polynomial $\phi(x)$. Then

$$\mathbf{f} = V \mathbf{a}, \quad V_{j,k} = t_j^k, \quad (6.4.17)$$

where V is a Vandermonde matrix. The set of derivatives $f^{(q)}(x)$ are then obtained by solving Eqs (6.4.17). This yields the quadrature rule

$$Q_\beta \left[m; n; \mathbf{t}^{(0)}; \mathbf{t}^{(1)} \right] \approx \int_0^1 f(x) e^{\beta x} dx, \quad (6.4.18)$$

which for $\beta = 2\pi il$ leads to formula (6.4.16).

Giunta and Murli (1987) consider the Fourier coefficients for a smooth function $f(x)$ on the interval $[a, b]$:

$$\begin{aligned} C^{(k)}(f) &= \frac{2}{b-a} \int_a^b f(x) \cos \frac{2k\pi(x-a)}{b-a} dx, \\ S^{(k)}(f) &= \frac{2}{b-a} \int_a^b f(x) \sin \frac{2k\pi(x-a)}{b-a} dx, \end{aligned} \quad (6.4.19)$$

and use the Lyness's algorithm as follows. For $f \in C^{(n)}[a, b]$, the early terms in the Euler expansion are $f(x) = h_{n-1}(x) + g_n(x)$, where $h_{n-1}(x) \in \mathcal{P}_{n-1}$ is defined by

$$h_{n-1}(x) = \sum_{q=1}^{n-1} \frac{1}{q!} \lambda_q B_q \left(\frac{x-a}{b-a} \right), \quad (6.4.20)$$

where $\lambda_q = [f^{(q-1)}(b) - f^{(q-1)}(a)] (b-a)^{q-1}$, and $B_q(x)$ are the Bernoulli polynomials. Then

$$C^{(k)}(f) = C^{(k)} h_{n-1} + C^{(k)} g_n, \quad S^{(k)}(f) = S^{(k)} h_{n-1} + S^{(k)} g_n, \quad (6.4.21)$$

with

$$\begin{aligned} C^{(0)} h_{n-1} &= S^{(0)} h_{n-1} = 0, \\ C^{(k)} h_{n-1} &= 2 \sum_{q=2}^{n-1} \text{E} \frac{(-1)^{q/2+1}}{(2\pi k)^q} \lambda_q, \quad k > 0, \\ S^{(k)} h_{n-1} &= 2 \sum_{q=1}^{n-1} \text{O} \frac{(-1)^{(q+1)/2}}{(2\pi k)^q} \lambda_q, \end{aligned}$$

where the superscript E or O restricts the values to even or odd values of the summation index. The Fourier coefficients of g_n , $C^{(k)}(f)$ and $S^{(k)}(f)$ are approximated by μ_k^n

and ν_k^m , respectively, where

$$\begin{aligned}\mu_0^m &= \frac{1}{b-a} T_x^{[m,1]}(g_n), \\ \mu_k^m &= \frac{2}{b-a} T_x^{[m,1]}\left(g_n \cos \frac{2k\pi(x-a)}{b-a}\right), \quad k < m/2, \\ \mu_{m/2}^m &= \frac{1}{b-a} T_x^{[m,1]}\left(g_n \cos \frac{m\pi(x-a)}{b-a}\right), \\ \nu_k^m &= \frac{2}{b-a} T_x^{[m,1]}\left(g_n \sin \frac{2k\pi(x-a)}{b-a}\right), \quad k \leq m/2, \\ \mu_k^m &= \nu_k^m = 0, \quad k > m/2,\end{aligned}\tag{6.4.22}$$

and $T_x^{[m,1]}$ denotes the m -panel trapezoidal rule on the interval $[a, b]$. A Fortran program FORCO containing subroutines is provided to implement an automatic version of the Lyness's algorithm.

6.5. Finite Fourier Transforms

When the domain of the physical problem is finite, it is generally not convenient to use the transforms with an infinite range of integration. In many cases finite Fourier transform can be used with advantage. We define

$$F_s(n) = \int_0^a f(x) \sin\left(\frac{n\pi x}{a}\right) dx \tag{6.5.1}$$

as the finite Fourier sine transform of $f(x)$. The function $f(x)$ is then given by

$$f(x) = \frac{2}{a} \sum_1^\infty F_s(n) \sin\left(\frac{n\pi x}{a}\right). \tag{6.5.2}$$

Similarly, the finite Fourier cosine transform is defined by

$$F_c(n) = \int_0^a f(x) \cos\left(\frac{n\pi x}{a}\right) dx, \tag{6.5.3}$$

and its inverse by

$$f(x) = \frac{F_c(0)}{a} + \frac{2}{a} \sum_1^\infty F_c(n) \cos\left(\frac{n\pi x}{a}\right). \tag{6.5.4}$$

EXAMPLE 6.5.1. Consider the Laplace equation in the rectangle $\{0 < x < a, 0 < y < b\}$

$$u_{xx} + u_{yy} = 0, \tag{6.5.5}$$

with the boundary conditions $u(0, y) = u(a, y) = u(x, b) = 0$ and $u(x, 0) = f(x)$. After applying the finite Fourier sine transform to $u(x, y)$ with respect to x from 0 to a , we have

$$\begin{aligned}(U_s)_{xx}(n) &= \int_0^a u_{xx} \sin \frac{n\pi x}{a} dx \\ &= \frac{n\pi}{a} [u(0, y) - (-1)^n u(a, y)] - \frac{n^2\pi^2}{a^2} U_s(n).\end{aligned}\tag{6.5.6}$$

Then Eq (6.5.5) becomes $\left[\frac{d^2}{dy^2} - \frac{n^2\pi^2}{a^2} \right] U_s(n, y) = 0$. Solving for $U_s(n, y)$, we get $U_s(n, y) = Ae^{n\pi y/a} + Be^{-n\pi y/a}$. Since $U_s(n, b) = 0$, we can express $U_s(n, y)$ as

$$U_s(n, y) = A_n \left(e^{n\pi(y-b)/a} - e^{-n\pi(y-b)/a} \right).$$

After applying the boundary condition at $y = 0$, we get

$$A_n \left(e^{-n\pi b/a} - e^{n\pi b/a} \right) = \bar{f}_s(n),$$

which, after solving for A_n and substituting its value into $U_s(n, y)$, yields $U_s(n, y) = -\frac{\sinh[n\pi(y-b)/a]}{\sinh(n\pi b/a)} \bar{f}_s(n)$. Hence,

$$u(x, y) = \frac{2}{a} \sum_1^\infty \frac{\sinh[n\pi(b-y)/a]}{\sinh(n\pi b/a)} \bar{f}_s(n) \sin(n\pi x/a),$$

where

$$\bar{f}_s(n) = \int_0^a f(\xi) \sin(n\pi\xi/a) d\xi. \blacksquare$$

EXAMPLE 6.5.2. Solve the wave equation $u_{tt} = c^2 u_{xx}$, $0 < x < l$, subject to the conditions $u(0, t) = g(t)$ and $u(l, t) = 0$ for $0 < x < l$, and $u(x, 0) = 0$ for $t > 0$. Taking the finite Fourier sine transform with respect to x and using the boundary conditions at $x = 0, l$, and (6.5.6), we get

$$\frac{d^2 U_s}{dt^2} + \frac{n^2\pi^2 c^2}{l^2} U_s = \frac{n\pi c^2}{l} g(t).$$

The general solution of this equation is

$$U_s(n) = A \cos \frac{n\pi ct}{l} + B \sin \frac{n\pi ct}{l} + U_{s,p}(n),$$

where $U_{s,p}(n)$ is the particular solution which can be obtained by the method of variation of parameters as

$$U_{s,p}(n) = c \int_0^t g(\tau) \sin \frac{n\pi c(t-\tau)}{l} d\tau = c \int_0^t g(t-\tau) \sin \frac{n\pi c\tau}{l} d\tau.$$

With this choice of $U_{s,p}(n)$, the constants A and B become zero because of the initial condition $U_s(n, 0) = 0$. Hence, $U_s(n) = U_{s,p}(n)$. Thus, by (6.5.2)

$$u(x, t) = \frac{2c}{l} \sum_{n=1}^{\infty} \sin \frac{n\pi x}{l} \int_0^t g(t-\tau) \sin \frac{n\pi c\tau}{l} d\tau. \blacksquare$$

Note that the finite cosine transforms for the derivatives of a function u can be obtained analogous to (6.5.6).

EXAMPLE 6.5.3. By using both Laplace and Fourier transforms, we will solve the boundary value problem

$$u_{tt} - c^2 u_{xx} = e^{-|x|} \sin t, \quad u(x, 0) = 0, \quad u_t(x, 0) = e^{-|x|}.$$

Note that this equation in the Laplace transform domain is

$$s^2 \bar{u}(x, s) - c^2 \bar{u}_{xx}(x, s) = \frac{2 + s^2}{1 + s^2} e^{-|x|}.$$

Applying the complex Fourier transform, we get

$$(c^2 \omega^2 + s^2) \bar{U}(x, s) = \frac{2 + s^2}{1 + s^2} \sqrt{\frac{2}{\pi}} \frac{1}{1 + \omega^2}.$$

Thus,

$$\begin{aligned} \bar{U}(x, s) &= \frac{2 + s^2}{1 + s^2} \sqrt{\frac{2}{\pi}} \frac{1}{(1 + \omega^2)(c^2 \omega^2 + s^2)} \\ &= \frac{2 + s^2}{(1 + s^2)(s^2 - c^2)} \sqrt{\frac{2}{\pi}} \left[\frac{1}{1 + \omega^2} - \frac{c^2}{c^2 \omega^2 + s^2} \right]. \end{aligned}$$

On inverting the Fourier transform, we have

$$\begin{aligned} \bar{u}(x, s) &= \frac{2 + s^2}{(1 + s^2)(s^2 - c^2)} \left(e^{-|x|} - \frac{c}{s} e^{-s|x|/c} \right) \\ &= \left\{ B \left(\frac{1}{s-c} - \frac{1}{s+c} \right) - \frac{1}{(1+c^2)(1+s^2)} \right\} e^{-|x|} \\ &\quad + \left\{ \frac{2}{cs} - B \left(\frac{1}{s-c} + \frac{1}{s+c} \right) - \frac{cs}{(1+c^2)(1+s^2)} \right\} e^{-s|x|/c}, \end{aligned}$$

where $B = \frac{2+c^2}{2c(1+c^2)}$. After taking the Laplace inverse, we find that

$$u(x, t) = \left[B (e^{ct} - e^{-ct}) - \frac{1}{1+c^2} \sin t \right] e^{-|x|} \\ + H(ct - |x|) \left[\frac{2}{c} - B (e^{ct-|x|} + e^{-ct+|x|}) - \frac{c}{1+c^2} \cos(t - |x|/c) \right]. \blacksquare$$

6.6. Discrete Fourier Transforms

The k -th coefficient c_k of a complex Fourier series for a function g of period P is given by

$$c_k = \frac{1}{P} \int_0^P g(x) e^{-2\pi i k x / P} dx,$$

which, by using Riemann sum method, can be approximated by

$$c_k \approx \frac{1}{P} \sum_{j=0}^{N-1} g(x_j) e^{-2\pi i k x_j / P} \frac{P}{N} = \frac{1}{N} \sum_{j=0}^{N-1} g\left(\frac{jP}{N}\right) e^{-2\pi i j k / N}, \quad (6.6.1)$$

where $x_j = j(P/N)$ denotes the left endpoint of the j -th subinterval for $j = 0, 1, \dots, N-1$. Thus, given N complex numbers, $\{f_j\}_{j=0}^{N-1}$, their N -point discrete Fourier transform (DFT), denoted by $\{F_k\}$, is given by

$$F_k = \sum_{j=0}^{N-1} f_j e^{-2\pi i j k / N} \quad (6.6.2)$$

for all integers $k = 0, \pm 1, \pm 2, \dots$. Note that it is a normal convention to use a lower-case letter for a given finite sequence of numbers and an upper-case version of the same letter for its DFT. As an example, let $f_j = e^{ja}$, for $j = 0, 1, \dots, N-1$, and a a constant. Then its N -point DFT is given by $F_k = \frac{1 - e^{aN}}{1 - e^{-a-2\pi i k / N}}$. The DFT is useful for approximating the coefficients c_k . Formula (6.6.1) leads to the fast Fourier transform (FFT) which, by grouping terms in (6.6.1), reduces the computation considerably.

Suppose the sequence $\{f_j\}_{j=0}^{N-1}$ has N -point DFT $\{F_k\}$ and $\{g_j\}_{j=0}^{N-1}$ has N -point DFT $\{G_k\}$. Then the basis properties of the DFT are:

(i) LINEARITY. For all complex numbers a and b , the sequence $\{af_j + bg_j\}_{j=0}^{N-1}$ has N -point DFT $\{aF_k + bG_k\}$.

(ii) PERIODICITY. For all integers k we have $F_{k+N} = F_k$.

(iii) INVERSION. For $j = 0, 1, \dots, N-1$, we have

$$f_j = \frac{1}{N} \sum_{k=0}^{N-1} F_k e^{2\pi i j k / N}. \quad (6.6.3)$$

The relationship between (6.6.2) and (6.6.3) can be expressed as

$$F_k \longleftrightarrow f_j, \quad (6.6.4)$$

where the sequence $\{f_j\}_{j=0}^{N-1}$ is the DFT of the sequence $\{F_k\}_{k=0}^{N-1}$. Functions related to each other by an integral Fourier transform will also be connected by the double-headed arrow, such that the function on the right is the Fourier integral transform of the one on the left. The sequence appearing on the right in (6.6.4) is usually a function of frequency and is known as the DFT of the sequence on the left, which is usually a function of time, space, or simply a sequential index and is known as the Fourier series or the inverse discrete Fourier transform (IDFT) of the sequence on the right, or sometimes simply as 'data'. An important property is that the indices of $F_k \longleftrightarrow f_j$ are interpreted modulo N ; however, F_{-k} for $0 \leq k < N-1$ is understood to mean F_{N-k} . Other useful definitions and properties are as follows.

(i) A sequence is even if $F_k = F_{-k}$, and odd if $F_k = -F_{-k}$. A sequence is conjugate even or conjugate odd if $F_k = F_{-k}^*$ or $F_k = -F_{-k}^*$, where the asterisk denotes the complex conjugate. A sequence is even or odd iff f_j is even or odd, respectively, i.e., $F_{-k} \longleftrightarrow f_{-j}$.

(ii) $F_k^* \longleftrightarrow f_{-j}^*$, and $F_{-k}^* \longleftrightarrow f_j$. Thus, F_k is real or imaginary iff f_j is conjugate even or conjugate odd, respectively, i.e., $f_j = \pm f_{-j}^*$. Moreover, f_j is real or imaginary iff F_k is even or odd, respectively, i.e., $F_k = \pm F_{-k}^*$.

(iii) F_k is real and even iff f_j is real and even; F_k is real and odd iff f_j is imaginary and odd; F_k is imaginary and even iff f_j is imaginary and even; F_k is imaginary and odd iff f_j is real and odd.

Let W denote either $e^{-2\pi i/N}$ or $e^{2\pi i/N}$. In either case we have $W = 1$. Thus, by periodicity, every DFT $\{F_k\}$ satisfies $F_{N-k} = F_{-k}$, and the Parseval's equality holds, i.e.,

$$\sum_{j=0}^{N-1} |f_j|^2 = \frac{1}{N} \sum_{k=0}^{N-1} |F_k|^2. \quad (6.6.5)$$

The approximation in (6.6.1) needs some interpretation. Since the right side of (6.6.1) is $1/N$ times the DFT of $\{g(jP/N)\}_{j=0}^{N-1}$ it has period N in the variable k . The left side of (6.6.1) is c_k , which does not have period N . Thus, to ensure that the sum (6.6.1) is valid we will assume that $|k| \leq N/8$.

In view of the approximation (6.6.1), we can write the M -th partial sum S_M of

the Fourier series of a function g of period P as

$$S_M(x) \approx \sum_{k=-M}^M \frac{1}{N} G_k e^{2\pi i k x / P}, \quad (6.6.6)$$

where $\{G_k\}$ is the N -point DFT of the sequence $\{g(jP/N)\}_{j=0}^{N-1}$. Substituting the sampling points $\{jP/N\}_{j=0}^{N-1}$ for x into (6.6.6), we obtain

$$S_M\left(\frac{jP}{N}\right) \approx \frac{1}{N} \sum_{k=-M}^M G_k e^{2\pi i j k / N}.$$

This formula can be expressed as an N -point (inverse) DFT with weight $W_N = e^{2\pi i / N}$, which is the N -th complex root of unity, if we use $G_{N-k} = G_{-k}$:

$$\begin{aligned} S_M\left(\frac{jP}{N}\right) &\approx \frac{1}{N} \sum_{k=0}^M G_k W_N^{jk} + \frac{1}{N} \sum_{k=1}^M G_{-k} W_N^{-jk} \\ &= \frac{1}{N} \sum_{k=0}^M G_k W_N^{jk} + \frac{1}{N} \sum_{k=1}^M G_{N-k} W_N^{j(N-k)} \\ &= \frac{1}{N} \sum_{k=0}^M G_k W_N^{jk} + \frac{1}{N} \sum_{k=N-M}^{N-1} G_k W_N^{jk}. \end{aligned} \quad (6.6.7)$$

If we define

$$F_k = \begin{cases} G_k & \text{for } k = 0, 1, \dots, M, \\ 0 & \text{for } k = M+1, \dots, N-M+1, \\ G_{N-k} & \text{for } k = N-M, \dots, N-1, \end{cases}$$

then we have

$$S_M\left(\frac{jP}{N}\right) \approx \frac{1}{N} \sum_{k=0}^{N-1} F_k W_N^{jk}, \quad (6.6.8)$$

which expresses the Fourier series partial sum values $\{S_M(jP/N)\}_{j=0}^{N-1}$ as the N -point DFT of $\{F_k\}$ with weight $W_N = e^{2\pi i / N}$, multiplied by $1/N$.

6.6.1. Discrete Sine and Cosine Transforms. Using the definitions in §6.1, the k -th sine coefficient B_k of a real-valued function g over the interval $[0, L]$ is defined by $B_k = \frac{2}{L} \int_0^L g(x) \sin \frac{k\pi x}{L} dx$, and the k -th cosine coefficient A_k by $A_k = \frac{2}{L} \int_0^L g(x) \cos \frac{k\pi x}{L} dx$. The discrete sine transform are obtained by approximating the integral for B_k by a uniform Riemann sum:

$$B_k \approx \frac{2}{L} \sum_{j=0}^{N-1} g\left(\frac{jL}{N}\right) \sin \frac{k\pi jL/N}{L} \frac{L}{N} = \frac{2}{N} \sum_{j=1}^{N-1} g\left(\frac{jL}{N}\right) \sin \frac{k\pi jL/N}{L}. \quad (6.6.9)$$

Similarly, we have

$$A_k \approx \frac{2}{N} \sum_{j=0}^{N-1} g\left(\frac{jL}{N}\right) \cos \frac{k\pi jL/N}{L}. \quad (6.6.10)$$

Hence, for a real sequence $\{f_j\}_{j=0}^{N-1}$ the *discrete sine transform* (DST), $\{F_k^S\}$, is defined by

$$F_k^S = \sum_{j=1}^{N-1} f_j \sin \frac{\pi jk}{N},$$

and the *discrete cosine transform* (DCT), $\{F_k^C\}$, by

$$F_k^C = \sum_{j=1}^{N-1} f_j \cos \frac{\pi jk}{N}.$$

The approximations (6.6.9) and (6.6.10) are valid only for $k \ll n$. Hence, we will henceforth assume that $k \leq n/4$.

If $S_M(x)$ denotes the M -harmonic partial sum of the Fourier sine series, then

$$S_M(x) = \sum_{k=1}^M B_k \sin \frac{k\pi x}{L},$$

where B_k are defined by (6.6.9). Assuming that $M \leq N/4$, we obtain the approximation

$$S_M(x) \approx \frac{2}{N} \sum_{k=1}^M G_k^S \sin \frac{k\pi x}{L},$$

where $\{G_k^S\}$ is the DST of $\{g(jL/N)\}$. If we replace x by the sample points jL/N , we get

$$\begin{aligned} S_M\left(\frac{jL}{N}\right) &\approx \frac{2}{N} \sum_{k=1}^M G_k^S \sin \frac{k\pi jk}{N}, \\ &= \frac{2}{N} \sum_{k=0}^M F_k^S \sin \frac{\pi jk}{L}, \quad j = 1, \dots, N-1, \end{aligned} \quad (6.6.11)$$

where the sequence $\{F_k^S\}$ is defined by

$$F_k^S = \begin{cases} G_k^S & \text{for } k = 1, \dots, M, \\ 0 & \text{for } k = M+1, \dots, N-1. \end{cases}$$

Similarly, we approximate Fourier cosine series and obtain

$$\begin{aligned} S_M\left(\frac{jL}{N}\right) &\approx \frac{2}{N} \left[\frac{1}{2} G_0^C + \sum_{k=1}^M G_k^C \cos \frac{k\pi jk}{N} \right], \\ &= \frac{2}{N} \sum_{k=0}^M F_k^C \cos \frac{\pi jk}{L}, \quad j = 1, \dots, N-1, \end{aligned} \quad (6.6.12)$$

where

$$F_k^C = \begin{cases} \frac{1}{2} G_0^C & \text{for } k = 0, \\ G_k^C & \text{for } k = 1, \dots, M, \\ 0 & \text{for } k = M+1, \dots, N-1. \end{cases}$$

6.6.2. Radix 2 FFT. Let $N = 2^r$, where r is a positive integer. We denote the N -point DFT by

$$F_k = \sum_{j=0}^{N-1} f_j W_N^{jk}, \quad (6.6.13)$$

where W_N is defined above.

FIRST STAGE. The FFT algorithm begins by halving this N -point DFT into two sums, each of which is a $N/2$ -point DFT:

$$F_k = \sum_{j=0}^{N/2-1} f_{2j} (W_N^2)^{jk} + \sum_{j=0}^{N/2-1} f_{2j+1} (W_N^2)^{jk} W_N^k, \quad (6.6.14)$$

which can also be written as

$$\begin{aligned} F_k &= F_k^0 + W_N^k F_k^1, \\ F_k^0 &= \sum_{j=0}^{N/2-1} f_{2j} (W_N^2)^{jk}, \\ F_k^1 &= \sum_{j=0}^{N/2-1} f_{2j+1} (W_N^2)^{jk}, \quad k = 0, 1, \dots, N-1. \end{aligned} \quad (6.6.15)$$

Note that the binary (base 2) expansion of the indices of f_0, f_2, \dots, f_{N-2} all end with 0 because the indices are even; thus, we have superscript 0 in $\{F_k^0\}$. Again, the binary expansions of the indices f_1, f_3, \dots, f_{N-1} all end in 1; thus, we have the superscript 1 in $\{F_k^1\}$. Using the prefix ‘DFT’ for ‘DFT of’, we can represent these superscripts as

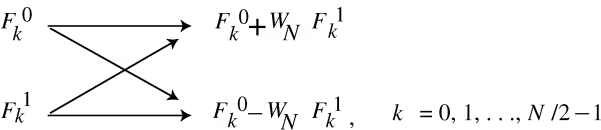
$$\{F_k^0\} = \text{DFT}\{f_{\dots 0}\}, \quad \{F_k^1\} = \text{DFT}\{f_{\dots 1}\}. \quad (6.6.16)$$

Since $N = 2^r$, we divide N evenly by 2, which gives $W_N^{N/2} = 1$, which lets us rewrite the first equation in (6.6.15) as

$$F_k = F_k^0 + W_N^k F_k^1, \quad F_{k+N/2} = F_k^0 - W_N^k F_k^1, \quad \text{for } k = 0, 1, \dots, N/2 - 1.$$

(6.6.17)

We can represent the computations in (6.6.17) by the following butterfly diagram:



There are $N/2$ butterflies at this stage of the FFT and each butterfly needs one multiplication which is $W_N^k \times F_k^1$. In Fig. 6.6.1 we have listed all the butterflies needed at this stage when $N = 2^4$. We can split $\{F_k\}$ into two half-size DFT's, $\{F_k^0\}$ and $\{F_k^1\}$, on $\{F_k^0\}$ and $\{F_k^1\}$ themselves, which yields

$$\begin{aligned} F_k^0 &= F_k^{00} + (W_N^2)^k F_k^{01}, & F_{k+N/4}^0 &= F_k^{00} - (W_N^2)^k F_k^{01}, \\ F_k^1 &= F_k^{10} + (W_N^2)^k F_k^{11}, & F_{k+N/4}^1 &= F_k^{10} - (W_N^2)^k F_k^{11}, \end{aligned}$$

(6.6.18)

for $k = 0, 1, \dots, N/4 - 1$.

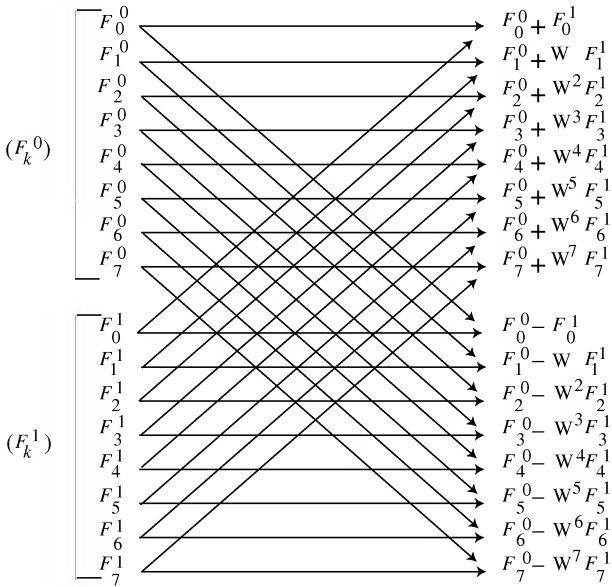


Fig. 6.6.1. First Reduction of FFT for $N = 2^4$.

Note that in (6.6.18) $\{F_k^{00}\}$ is the $\frac{N}{4}$ -point DFT of $\{f_0, f_4, f_8, \dots, f_{N-4}\}$, $\{F_k^{01}\}$ the $\frac{N}{4}$ -point DFT of $\{f_2, f_6, \dots, f_{N-2}\}$, $\{F_k^{10}\}$ the $\frac{N}{4}$ -point DFT of $\{f_1, f_5, \dots, f_{N-3}\}$,

and $\{F_k^{11}\}$ the $\frac{N}{4}$ -point DFT of $\{f_3, f_7, \dots, f_{N-1}\}$. This is represented in terms of the binary expressions of f_j by

$$\begin{aligned}\{F_k^{00}\} &= \text{DFT} \{f_{\dots 00}\}; & \{F_k^{01}\} &= \text{DFT} \{f_{\dots 10}\}; \\ \{F_k^{10}\} &= \text{DFT} \{f_{\dots 01}\}; & \{F_k^{11}\} &= \text{DFT} \{f_{\dots 11}\}.\end{aligned}$$

There is a reversal of the last two digits (bits) in the above binary expansions of the indices j in $\{f_j\}$ for which we compute the $\frac{N}{4}$ -point DFTs $\{F_k^{00}\}$, $\{F_k^{01}\}$, $\{F_k^{10}\}$, and $\{F_k^{11}\}$. The two stages of the FFT are presented in Fig. 6.6.2.

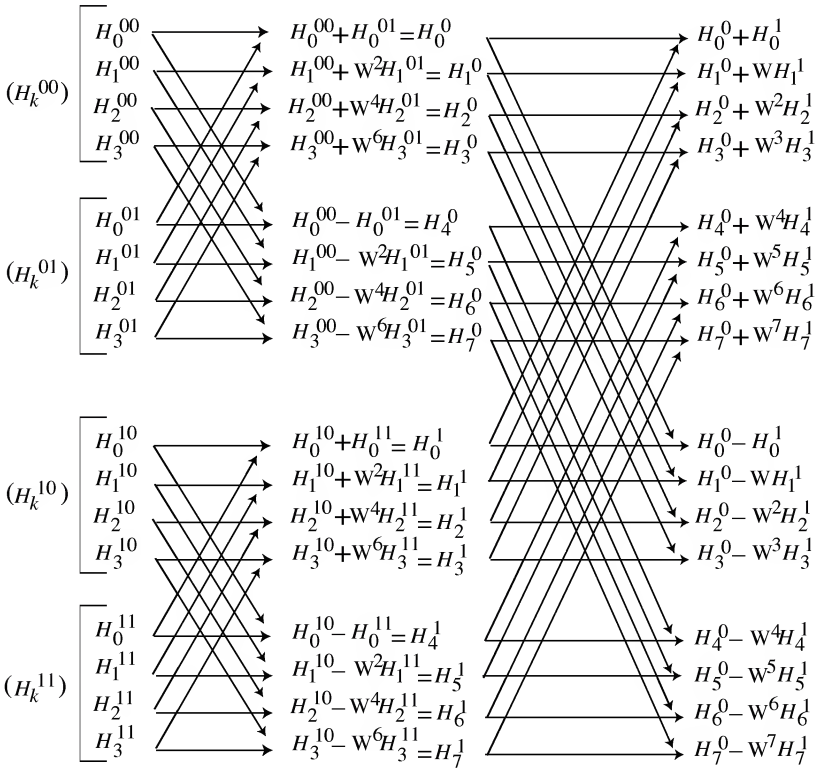


Fig. 6.6.2. Two Stages of FFT for $N = 4^2$.

If this process is continued by halving the order of the DFTs, then after $\log_2 N$ stages we arrive at a point where we are performing N one-point DFTs, which for a number f_j is the identity $f_j \rightarrow f_j$. Since the process of indexing the smaller size DFTs by subscripts where the reversing order of the bits in the indices of $\{f_j\}$ continues, it so happens that by the time the one-point stage is reached all bits in the binary expansion of j are arranged in the reverse order, as shown in Fig. 6.6.3. Hence, the FFT computation is started by first rearranging $\{f_j\}$ so that it is listed in

bit reverse order.

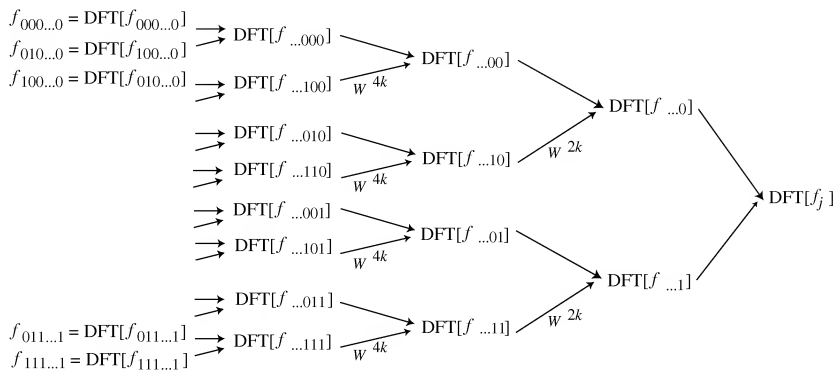


Fig. 6.6.3. Reduction of FFT and Bit Reversal.

The main components of the FFT are: (i) bit reversal reordering of the initial data; (ii) rotations involved in the butterfly computations; and (iii) computation of the sines need for (ii). The savings in the computer time with FFT are enormous. For each of the $\log_2 N$ stages there are $N/2$ multiplications; thus the total number of multiplications needed for the FFT are $\frac{1}{2} \log_2 N$, as compared to the direct computation of DFT which takes $(N - 1)^2$ multiplications. For example, for $N = 2^{10}$, the FFT requires 5120 multiplications whereas the direct DFT will require 1 046 529 multiplications, which means that in FFT the saving in multiplication time is by a factor of about 204.

Bunemann’s algorithm performs the bit reversal permutation as follows: If the N numbers $\{0, 1, \dots, N - 1\}$ are permuted by bit reversing their binary expansions, then the permutation of $2N$ numbers $\{0, 1, \dots, 2N - 1\}$ is obtained by doubling the numbers in the permutation of $\{0, 1, \dots, N - 1\}$ to get the first N numbers and then adding 1 to these doubled numbers to get the last N numbers.

Table 6.6.1.

r	$r/\log_2 r$	r	$r/\log_2 r$	r	$r/\log_2 r$
2	2.00	5	2.15	8	2.67
3	1.88	6	2.31	9	2.87
4	2.00	7	2.49	10	3.01

MINIMIZATION OF NUMBER OF OPERATIONS. The number of operations (additions and multiplications) for N -point Fourier analysis is N^2 . By factoring $N = r \times s$, the number of operations $= r^2s + s^2r = N \times (r + s)$. In general, by factoring $N = r_1 \times r_2 \times \dots \times r_m$, the number of operations $= N \times (r_1 + r_2 + \dots + r_m)$. For a minimum, $r_1 = \dots = r_m = r$, $N = r^m$, i.e., $m = \log_r N$, the number of operations

$= N \cdot r \cdot \log_r N = N \cdot \log_2 N \cdot \frac{r}{\log_2 r}$. Table 6.6.1 represents the value of $\log_2 r$ for $r = 2, \dots, 10$. For additional information on DFT and bit reversal permutation, see [BitReversalAlgorithms.pdf](#) on the CD-R; for Bracewell-Bunemann code see [fft.f90](#) and [BracewellBunemann.nb](#) on the CD-R;

6.6.3. FFT Procedures. Assuming that a Fourier series subroutine exists such that its input is the complex sequence f_j , $j = 0, 1, \dots, N-1$, and output the Fourier series (or IDFT) F_k defined by (6.6.2), Cooley et al. (1970) have described the following seven FFT procedures that are based on the FFT algorithm (§6.6.4).

PROCEDURE 1. FOURIER TRANSFORM. Let F_k^*/N replace f_j as input and f_j^* replace F_k as output. Then the subroutine (6.6.3) will compute the DFT f_j .

PROCEDURE 2. FOURIER TRANSFORM OF TWO SETS OF REAL DATA IN ONE PASS THROUGH A DFT SUBROUTINE. If F_k^1 and F_k^2 are real sequences such that $F_k^1 \longleftrightarrow f_j^1$, $F_k^2 \longleftrightarrow f_j^2$, and $F_k = F_k^1 + i F_k^2$, then, by the linearity property, F_k has the transform $f_j = f_j^1 + i f_j^2$. Replacing j by $N-j$ and taking complex conjugates of both sides, we get $f_{N-j}^* = f_j^1 - i f_j^2$. Solving these two relations for f_j^1 and f_j^2 we obtain

$$f_j^1 = \frac{1}{2} [f_{N-j}^* + f_j], \quad f_j^2 = \frac{i}{2} [f_{N-j}^* - f_j]. \quad (6.6.19)$$

Thus, Procedure 2 is: (a) form F_k as defined by $F_k = F_k^1 + i F_k^2$; (b) compute f_j by means of the DFT subroutine; and (c) compute f_j^1 and f_j^2 by (6.6.19) for $j = 0, 1, \dots, N/2$.

PROCEDURE 3. DOUBLING ALGORITHM FOR COMPUTING FOURIER TRANSFORM OF $2N$ POINTS FROM THE TRANSFORMS OF TWO N -POINT SEQUENCES. Given $2N$ data points Y_k with $Y_k \longleftrightarrow y_j$ for $j, k = 0, 1, \dots, 2N-1$, suppose the two N -point sequences $F_k^1 = Y_{2k}$ and $F_k^2 = Y_{2k+1}$, $k = 0, 1, \dots, N-1$, have the N -point transforms f_j^1 and f_j^2 such that $F_k^1 \longleftrightarrow f_j^1$ and $F_k^2 \longleftrightarrow f_j^2$, respectively. Separating the even- and odd-indexed points in the series for y_j , we have

$$\begin{aligned} y_j &= \frac{1}{2N} \sum_{k=0}^{2N-1} Y_k W_{2N}^{-jk} = \frac{1}{2N} \left\{ \sum_{k=0}^{N-1} Y_{2k} W_{2N}^{-2jk} + \sum_{k=0}^{N-1} Y_{2k+1} W_{2N}^{-2jk-j} \right\} \\ &= \frac{1}{2N} \left\{ \sum_{k=0}^{N-1} Y_{2k} W_N^{-jk} + \sum_{k=0}^{N-1} Y_{2k+1} W_N^{-jk} W_{2N}^{-j} \right\}, \quad \text{since } W_{2N} = W_N, \end{aligned}$$

in which the summations define f_j^1 and f_j^2 , respectively, so we can write y_j as

$$y_j = \frac{1}{2} [f_j^1 + f_j^2 W_{2N}^{-j}]. \quad (6.6.20)$$

Substituting $N+j$ for j and using the fact that $W_{2N}^N = -1$, we get

$$y_{N+j} = \frac{1}{2} [f_j^1 - f_j^2 W_{2N}^{-j}]. \quad (6.6.21)$$

Thus, Procedure 3 is: (a) compute the two N -point DFT's of the sequences $F_k^1 = F_{2k}$ and $F_k^2 = F_{2k+1}$; and
(b) apply (6.6.20) and (6.6.21) to the resulting transform.

This procedure, when iterated upon to produce successive doublings up to N , which is the total number of points, is the FFT algorithm with radix 2, as described in §6.6.2.

PROCEDURE 4. COMPUTATION OF THE DFT OF REAL DATA. Using Procedures 2 and 3, the transform of a single sequence of $2N$ real data points is computed by one DFT of N complex points. The details are as follows. First, assume that Y_k , $k = 0, 1, \dots, N-1$, is the real sequence, and let $Y_k \longleftrightarrow y_j$. Then, form the N -point sequences

$$F_k^1 = Y_{2k}, \quad F_k^2 = Y_{2k+1}, \quad F_k = F_k^1 + i F_k^2. \quad (6.6.22)$$

Compute the N -point Fourier transform of F_k and use Eq (6.6.19) to obtain the transform of the two real sequences F_k^1 , F_k^2 in terms of the DFT of F_k ; then use Procedure 3 and Eq (6.6.20) to obtain the transform of the entire array Y_k . Since Y_k is real, it means that the upper half of the y_j array is redundant; thus, $y_j = y_{2N-j}^*$. Since F_k^1 and F_k^2 are real, f_j^1 and f_j^2 are conjugate even. Then, replacing N by $N+j$ in (6.6.20) we obtain

$$y_{N+j} = \frac{1}{2} \left[f_j^1 - f_j^2 W_{2N}^{-j} \right]. \quad (6.6.23)$$

We can effectively use (6.6.20) and (6.6.23) for $j = 0, 1, \dots, N/2$. It can be easily seen that the coefficients y_j in $Y_k = \sum_{j=0}^{2N-1} y_j W_{2N}^{jk}$, $k = 0, 1, \dots, 2N-1$, are the sine-cosine coefficients of the series

$$Y_k = \frac{1}{2} a_0 + \sum_{j=1}^{N-1} \left\{ a_j \cos \frac{\pi j k}{N} + b_j \sin \frac{\pi j k}{N} \right\} + \frac{1}{2} (-1)^k a_N,$$

where $a_j = 2\Re\{y_j\}$ for $0 \leq j < N$, and $b_j = -2\Im\{y_j\}$ for $0 < j < N$. Thus, Procedure 4 is: (a) let the $2N$ -point array Y_k be put in a complex N -point array F_k as defined in (6.6.22);

(b) compute the N -point DFT of F_k ;

(c) use Eq (6.6.19) for $j = 0, 1, \dots, N/2$ to get f_j^1 and f_j^2 ; and

(d) apply Eqs (6.6.20) and (6.6.23) for $j = 0, 1, \dots, N/2$ to get y_j for $j = 0, 1, \dots, N$.

PROCEDURE 5. COMPUTATION OF FOURIER SERIES FOR REAL DATA. This is performed by reversing Procedure 4. The details are as follows. Solve (6.6.20) and (6.6.23) for f_j^1 and f_j^2 in terms of y_j and y_{N+j} , i.e.,

$$f_j^1 = y_j + y_{N+j}, \quad (6.6.24)$$

$$f_j^2 = [y_j - y_{N+j}] W_{2N}^j. \quad (6.6.25)$$

Then solve (6.6.19) to obtain

$$f_j = f_j^1 + i f_j^2, \quad (6.6.26)$$

$$f_{N-j}^* = f_j^1 - i f_j^2. \quad (6.6.27)$$

Thus, Procedure 5 is: (a) use (6.6.24) and (6.6.25) to generate f_j^1 and f_j^2 for $j = 0, 1, \dots, N/2$; (b) use (6.6.26) and (6.6.27) to generate f_j for $j = 0, 1, \dots, N/2$; and (c) compute the IDFT of the N -element complex array f_j . The result will be the sequence F_k whose real and imaginary parts are the real elements of Y_k as defined by (6.6.22).

We can also use Procedures 4 and 5 to transform a conjugate even data sequence F_k to a real frequency sequence f_j , and conversely, by letting F_k/N^* replace f_j and f_j^* replace F_k , thus switching the roles of ‘frequency’ and ‘data’.

PROCEDURE 6. COMPUTATION OF COSINE SERIES FOR REAL DATA. Since Y_k are real and even, its IDFT will be a cosine series. Thus, if $Y_k, k = 0, 1, \dots, 2N-1$, is real and $Y_k = Y_{2N-k}$, then

$$Y_k = \sum_{j=0}^{2N-1} y_j W_{2N}^{jk} = \frac{1}{2} a_0 + \sum_{j=1}^{N-1} a_j \cos \frac{\pi j k}{N} + \frac{1}{2} (-1)^k a_N,$$

where a_j are real and $a_j = 2y_j$. Thus, the DFT of Y_k can be written as a cosine series

$$y_j = \frac{2}{N} \left[\frac{1}{2} Y_0 + \sum_{k=1}^{N-1} Y_k \cos \frac{\pi j k}{N} + \frac{1}{2} (-1)^k Y_N \right].$$

To derive the procedure for computing a cosine transform of real data $Y_k, k = 0, 1, \dots, 2N-1$, such that $Y_{2N-k} = Y_k$, we only require Y_0, \dots, Y_N . First, define the complex sequence

$$F_k = Y_{2k} + i [Y_{2k+1} - Y_{2k-1}] \quad \text{for } k = 0, 1, \dots, N-1, \quad (6.6.28)$$

where we actually need to form only terms with $k = 0, 1, \dots, N/2$, since being a complex even sequence, its transform f_j must be real. Procedure 5 is an efficient method to transform a conjugate even sequence to a real sequence. Thus, let the conjugate even sequence F_k^*/N be the input to Procedure 5, and the output will be f_j , which is the real DFT of F_k . Once f_j is obtained, use Procedure 2 to obtain the transforms of real and imaginary parts of F_k . Thus, define $Y_{2k} \longleftrightarrow f_j^1, Y_{2k+1} \longleftrightarrow f_j^2$, and $Y_{2k}' = Y_{2k+1} - Y_{2k-1} \longleftrightarrow f_j^{2'}$. Use Eq (6.6.19), remembering that f_j is real, to get

$$f_j^1 = \frac{1}{2} [f_j + f_{-j}], \quad f_j^{2'} = \frac{1}{2i} [f_j - f_{-j}], \quad (6.6.29)$$

and derive $Y_{2k-1} \longleftrightarrow W_N^{-j} f_j^2$, which gives

$$f_j^{2'} = f_j^2 - W_N^{-j} f_j^2, \quad (6.6.30)$$

i.e., $f_j^2 = \frac{f_j^{2'}}{1 - W_N^{-j}}$. Next, we need to compute

$$f_0^2 = \sum_{k=0}^{N-1} Y_{2k+1}. \quad (6.6.31)$$

Finally, Procedure 3 takes us from f_j^1 and f_j^2 to y_j , which is the DFT of Y_k . Thus, substituting (6.6.29) and (6.6.30) into Eq (6.6.20), we get

$$a_j = 2y_j = \frac{1}{2} \left\{ [f_j + f_{-j}] - \frac{f_j - f_{-j}}{2 \sin(\pi j/N)} \right\}, \quad j = 1, 2, \dots, N-1, \quad (6.6.32)$$

where for $j = 0$ and $j = N$ we use

$$y_0 = \frac{1}{2} [f_0^1 + f_0^2], \quad y_N = \frac{1}{2} [f_0^1 - f_0^2]. \quad (6.6.33)$$

Thus, Procedure 6 is: (a) given the real even sequence Y_k for $k = 0, 1, \dots, 2N-1$, define F_k by (6.6.28);

(b) let F_k^*/N be the input to Procedure 5; the output will be $f_j^* = f_j$;

(c) compute y_j using (6.6.32) for $j = 1, 2, \dots, N-1$; let $f_0^1 = f_0$ and compute f_0^2 by (6.6.31); then use (6.6.33) to get y_0 and y_N ; finally, let $a_j = 2y_j$ for $j = 0, 1, \dots, N$.

PROCEDURE 7. COMPUTATION OF SINE SERIES FOR REAL DATA. If Y_k , $k = 0, 1, \dots, 2N-1$, is real and odd, it can be expressed as a sine series

$$Y_k = \sum_{j=0}^{2N-1} y_j W_{2N}^{jk} = \sum_{j=1}^{2N-1} b_j \sin \frac{\pi j k}{N},$$

where b_j are real and $b_j = 2i y_j$. Since $Y_0 = Y_N = 0$, we find that

$$b_j = \frac{2}{N} \sum_{k=1}^{N-1} Y_k \sin \frac{\pi j k}{N}.$$

Since Y_k is real and odd, iY_k is conjugate even, so its transform is real. Thus, $Y_k \longleftrightarrow y_j = b_j/(2i)$, and $iY_k \longleftrightarrow i y_j = \frac{1}{2} b_j$. Hence, if we let

$$F_k = -[Y_{2k+1} - Y_{2k-1}] + i Y_{2k}, \quad (6.6.34)$$

and use the same method as in deriving (6.6.32), we obtain

$$b_j = 2i y_j = \frac{1}{2} \left\{ [f_j - f_{-j}] - \frac{f_j - f_{-j}}{2 \sin(\pi j/N)} \right\}, \quad j = 1, 2, \dots, N-1. \quad (6.6.35)$$

Thus, Procedure 7 is: (a) given the values Y_k , $k = 0, 1, \dots, N-1$, of a real odd sequence Y_k , $k = 0, 1, \dots, 2N-1$, form F_k by (6.6.34);
 (b) let F_k^*/N be the input to Procedure 5; the output will be $f_j^* = f_j$;
 (c) compute b_j using (6.6.35) for $j = 1, 2, \dots, N-1$.

Note that Procedures 6 and 7 provide a four-fold decrease in computation and storage requirements since only one-half of the real input data arrays need be supplied. The complex data F_k to be transformed contains only $N/2$ terms rather than $2N$ required if full array Y_k is supplied for a complex DFT subroutine.

The effect of sampling of a function $f(t)$ at finite interval leads to the evaluation of $f(t)$ at the points $t_k = k \Delta t$, $k = 0, \pm 1, \pm 2, \dots$, with $T = 1/\Delta t$, by

$$f(t_k) = \int_{-\infty}^{\infty} F(\omega) e^{2i\pi k\omega/T} d\omega = \sum_{k=-\infty}^{\infty} \int_{kT}^{(k+1)T} F(\omega) e^{2i\pi k\omega/T} d\omega.$$

Since the exponential factor $e^{2i\pi k\omega/T}$ is periodic in ω with period P , the above relation can be written as

$$f(k\Delta t) = \int_0^P F^{(P)}(\omega) e^{2i\pi k\omega/P} d\omega,$$

where $F^{(P)}(\omega) = \sum_{j=-\infty}^{\infty} F(\omega + jP)$ is the periodized function $F(\omega)$, defined by

$$F^{(P)}(\omega) = \frac{1}{P} \sum_{k=-\infty}^{\infty} f(k\Delta t) e^{-2i\pi k\omega/P}. \quad (6.6.36)$$

The effect of sampling in the frequency domain at the points ω_n , $n = 0, \pm 1, \pm 2, \dots$, $\Delta\omega = 1/T$, we can rewrite (6.6.36) as

$$F^{(P)}(n\Delta\omega) = \frac{1}{P} \sum_{k=-\infty}^{\infty} f(k\Delta t) e^{-2i\pi nk/N},$$

where $N = TP$, and $f(k\Delta t) = \sum_{j=-\infty}^{\infty} f((k + jN)\Delta t)$. This represents the sample values of $F^{(P)}(t) = \sum_{j=-\infty}^{\infty} f(t + jT)$, which is a periodic function of t with period T . Thus, substituting T/N in place of $1/P$ in (6.6.36), we get

$$F^{(P)}(n\Delta\omega) = \frac{1}{N} \sum_{k=0}^{N-1} T f_p(k\Delta t) e^{-2i\pi kn/N}.$$

This relation can be represented in the form (6.6.4) if we let $h_j = T f_p(k\Delta t)$ and $H_k = F^{(P)}(n\Delta\omega)$. This proves the following result.

THEOREM 6.6.1. (Cooley et al. 1970) If $f(t) \longleftrightarrow F(\omega)$, then

$$T f_p(k\Delta t) \longleftrightarrow F^{(P)}(n\Delta\omega) \quad \text{for } k, n = 0, 1, \dots, N-1. \quad (6.6.37)$$

6.6.4. FFT Algorithm. The actual computation of the finite Fourier transforms has many applications. Although the number of data points must be finite, it can be very large on the order of 10^3 or 10^4 , which requires a considerable amount of computer time. An algorithm for this purpose that involves a drastic reduction in the computation, by a factor of $N/\log_2 N$, was developed by Cooley and Tukey (1965).

6.6.5. Linear Multistep Method. By using the Björck-Pereyra algorithm and FFT techniques we obtain some quadrature rules to approximate the finite range integrals of the form $\int_0^T (nh - x)^{-1/2} f(x) dx$, where h denotes the step size, and $T = nh$, $n = 1, 2, \dots, N$; $N = 2^R$, $R \in \mathbb{Z}^+$. These rules are derived from approximations to $I_0^T(f)$, which are generated by the implicit linear multistep method (LMM). These formulas provide good accuracy for functions f of the form $f(x) = f_0 + f_1 x^{1/2} + f_2 x + f_3 x^{3/2} + f_4 x^2 + \dots$ as $x \rightarrow 0$, with suitable 'starting' weights. A Fortran code is available in Baker and Derakhshan (1987).

We use the k -step method, which is used in initial value problems in ordinary differential equations, and consider the approximation

$$\int_0^{nh} f(x) dx \approx h \sum_{j=0}^n w_{nj} f(jh), \quad n \geq k, \quad (6.6.38)$$

where w_{nj} , $j = 0, 1, \dots, k-1$, are determined by the starting approximation for $\int_0^{nh} f(x) dx$, $n = 0, 1, \dots, k-1$, and are defined by

$$w_{nj} = \omega_{n-j}, \quad j = k, k+1, \dots, n,$$

where $\omega_0, \omega_1, \dots$, are the coefficients in the expansion of

$$\omega(\mu) = \frac{\sigma(\mu^{-1})}{\rho(\mu^{-1})} = \omega_0 + \omega_1 \mu + \omega_2 \mu^2 + \dots,$$

and

$$\begin{aligned} \rho(\mu) &= \alpha_0 \mu^k + \alpha_1 \mu^{k-1} + \dots + \alpha_k, \\ \sigma(\mu) &= \beta_0 \mu^k + \beta_1 \mu^{k-1} + \dots + \beta_k, \quad \beta \neq 0, \end{aligned}$$

denote the first and second characteristic polynomials in the LMM. This leads to the formula

$$\frac{1}{\sqrt{\pi}} \int_0^{nh} (nh - x)^{-1/2} f(x) dx \approx \sqrt{h} \sum_{j=0}^n W_{nj}^{(1/2)} f(jh), \quad (6.6.39)$$

where $W_{nj}^{(1/2)} = \Omega_{n-j}^{(1/2)}$, and

$$\Omega^{(1/2)}(\mu) = \{\omega(\mu)\}^{1/2} = \Omega_0^{(1/2)} + \Omega_1^{(1/2)} \mu + \Omega_2^{(1/2)} \mu^2 + \cdots. \quad (6.6.40)$$

For a suitable choice of the ‘starting’ weights $W_{nj}^{(1/2)}$, $j = 0, 1, \dots, 2p - 2$, is made to ensure that approximations (6.6.39) are of order p for the class of functions $f(x) = f_0 + f_1 x^{1/2} + f_2 x + f_3 x^{3/2} + f_4 x^2 + \cdots + F(x)$, where $F(x)$ is smooth.

The role of FFT involves the computation of the coefficients of a product of two polynomials. Thus, if $u(x) = \sum_{i=0}^{n-1} u_i x^i$ and $v(x) = \sum_{i=0}^{n-1} v_i x^i$ denote two polynomials, then their product $p(x) = u(x)v(x) = \sum_{i=0}^{2n-2} p_i x^i$ has the coefficients

$$p_m = \sum_{j=0}^m u_j v_{m-j}, \quad m = 0, 1, \dots, 2n - 2. \quad (6.6.41)$$

The FFT technique is used to compute these coefficients p_m as follows:

Let $\{u_0, u_1, \dots, u_{n-1}, 0, \dots, 0\}$ and $\{v_0, v_1, \dots, v_{n-1}, 0, \dots, 0\}$ be two sequences, each with 2^n elements, where $n = 2^{m-1}$, $m \in \mathbb{Z}^+$, and let $\{U_0, U_1, \dots, U_{2n-1}\}$ and $\{V_0, V_1, \dots, V_{2n-1}\}$ denote the two sequences that are obtained after computing the DFTs of the above two sequences; i.e.,

$$U_k = \frac{1}{\sqrt{2n}} \sum_{j=0}^{2n-1} u_j e^{-i\pi jk/n}, \quad (6.6.42)$$

and similar expression for V_k . Then,

$$p_k = \frac{1}{2n} \sum_{j=0}^{2n-1} V_j D_j e^{-i\pi jk/n}, \quad k = 0, 1, \dots, 2n - 2. \quad (6.6.43)$$

The transformations from $\{u_j\}$ to $\{U_k\}$, $\{v_j\}$ to $\{V_k\}$, and $\{V_k U_k\}$ to $\{p_j\}$ are carried out by fast routines such as C06FAF, C06GBF and C06FBF, available in the NAG library, which compute a transform, conjugate of a Hermitian sequence, and an inverse transform, respectively.

Thus, using (6.6.39), we compute a finite number of the coefficients $\Omega_j^{(1/2)}$, $j = 0, 1, 2, \dots$, in the formal power series (6.6.40) by the above FFT technique. Let $[\Omega^{(1/2)}(\mu)]_N = \sum_{j=0}^{N-1} \Omega_j^{(1/2)} \mu^j$ denote the *truncated* formal power series (6.6.40).

Then the sequence $\{\Omega_0^{(1/2)}, \Omega_1^{(1/2)}, \dots, \Omega_{N-1}^{(1/2)}\}$ is computed. It defines $[\Omega^{(1/2)}(\mu)]_N$ for $N = 2^R$, $R \in \mathbb{Z}^+$. Once this sequence is computed, we solve the system of linear equations in order to determine the starting weights $W_{nj}^{(1/2)}$ for $j = 0, 1, \dots, 2p - 2$,

which is done by using the formula

$$\begin{aligned} \frac{1}{\sqrt{\pi}} \int_0^{nh} (nh - x)^{-1/2} f(x) dx - \sqrt{h} \sum_{j=0}^n W_{nj}^{(1/2)} f(jh) \\ = O(hp) \quad \text{as } h \rightarrow 0, \end{aligned} \quad (6.6.44)$$

with $nh = T$ fixed, for any $f(x) = f_0 + f_1 x^{1/2} + f_2 x + f_3 x^{3/2} + f_4 x^2 + \cdots + f_{2p-3} x^{p-3/2} + f_{2p-2} x^{p-1} + F(x)$, where $F(x) \in C^p[0, T]$, and then solving the system of equations

$$\begin{aligned} \sqrt{h} \sum_{j=0}^{2p-2} W_{nj}^{(1/2)} (jh)^{m/2} = \frac{1}{\sqrt{\pi}} \int_0^{nh} (nh - x)^{-1/2} x^{m/2} dx \\ - \sqrt{h} \sum_{j=2p-1}^n \Omega_{n-j}^{(1/2)} (jh)^{m/2}, \quad \text{for } m = 0, 1, \dots, 2p-2. \end{aligned} \quad (6.6.45)$$

6.6.6. Computation of Fourier Coefficients. As Lyness (1987) has noted, the term ‘FFT’ describes both a series of methods and a series of computer codes to rapidly evaluate transform approximations. We will discuss how an FFT may be used to obtain approximations to Fourier coefficients.

For Fourier cosine and sine coefficients of a real function, we provide an even integer m as radix 2, with m items of data $\{a_0, a_1, \dots, a_{m/2}, b_0, b_1, \dots, b_{m/2-1}\}$, defined by

$$\begin{cases} a_s = \frac{2}{m} \sum_{k=0}^{m-1} d_k \cos 2\pi ks/m, & s = 0, 1, \dots, m/2; \\ b_s = \frac{2}{m} \sum_{k=0}^{m-1} d_k \sin 2\pi ks/m, & s = 0, 1, \dots, m/2 - 1. \end{cases} \quad (6.6.46)$$

Then what an FFT program does is simply as follows: The code involves a matrix multiplication of an $m \times m$ matrix whose elements are either $\cos 2\pi ks/m$ or $\sin 2\pi ks/m$. If coded as it is, this involves m^2 multiplications and m^2 additions. But it can be coded so that it involves only $\log_2 m$ multiplications. When m is very large (say, 2^{10}), it saves time in data manipulation by a larger factor (of 100). When m is small (say, 2^4), the relative time saving factor is much smaller (of 4). But only data manipulation time is reduced; the time spent on computation of function values d_k or processing the output a_s, b_s remains the same.

Let

$$\begin{aligned} d_0 &= \frac{1}{2} [f(a) + f(b)], \\ d_k &= f\left(a + \frac{k(b-a)}{m}\right) = f(x_k), \quad k = 1, 2, \dots, m-1. \end{aligned}$$

Then the FFT routine yields the quantities

$$\begin{aligned} a_s + i b_s &= \frac{2}{m} \sum_{k=0}^{m-1} f\left(a + \frac{k(b-a)}{m}\right) e^{2\pi i k s / m} \\ &= \frac{2 e^{-(2\pi i s a)/(b-a)}}{b-a} \left[\frac{b-a}{m} \sum_{k=0}^{m-1} f(x_k) e^{2\pi i s x_k / (b-a)} \right]. \end{aligned} \quad (6.6.47)$$

The quantity within the square brackets is the m -panel trapezoidal rule for the approximation of the integral representation of the Fourier coefficients, which is $\int_a^b f(x) e^{2\pi i s x / (b-a)} dx$ for $s = 0, 1, \dots, m/2$. This provides a very useful FFT routine if we have the $m+1$ equally spaced function values and seek to compute a set of m real (or $m/2$ complex) Fourier coefficients using the trapezoidal rule.

6.6.7. Filon-Luke Rule. Once the Fourier coefficients are computed by FFT, we take $\beta = 2\pi i s / (mh)$ and M panels, each having $d+1$ nodes. This requires $d+1$ (possibly d) sums of the form

$$\sum_{k=0}^{M-1} f(a + kh + x_j) e^{2\pi i s (a + kh) / (Mh)}, \quad (6.6.48)$$

where s is an integer. For the j -th sum of this form, we set $d_k = f(a + kh + x_j)$, $k = 0, 1, \dots, M-1$, in the FFT routine, which returns a_s and b_s (given by (6.6.47) with m replaced by M). Then the sum (6.6.48) becomes equal to

$$\frac{M}{2} (a_s + i b_s) e^{2\pi i s a / (Mh)}.$$

Some minor modifications are needed if $x_j = 0$ or h . The FFT routine defined in Giunta and Murli (1987) and Lyness (1974, 1984) are useful for this purpose.

6.7. Hartley Transform

The FFT requires a large computer time, but the fast Hartley transform (FHT) can get the same results only faster, as shown by Bracewell (1986). The Fourier transform maps a real function of time $f(t)$ onto a complex function of frequency $F(\omega)$, and it requires many arithmetical operations of complex multiplication or division, and two for complex addition or multiplication. But the Hartley transform maps a real function of time $f(t)$ onto a real function of frequency $H(\omega)$, where the Hartley frequency is real, and thus it needs only single arithmetical operations to compute it. Since the real data needs only half of the memory storage required for the complex data, the Hartley transform takes considerably less memory for a given set of data than the Fourier transform.

The Hartley transform and its inverse are defined by

$$H(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) \operatorname{cas}(2\pi\omega t) dt, \quad (6.7.1a)$$

$$f(t) = \int_{-\infty}^{\infty} H(\omega) \operatorname{cas}(2\pi\omega t) d\omega, \quad (6.7.1b)$$

where $\operatorname{cas}(\theta) = \cos(\theta) + \sin(\theta)$, a notation which was introduced by Hartley (1942). The complementary function of $\operatorname{cas}(t)$ is $\cos t - \sin t = \operatorname{cas}(-t) = \operatorname{cas}'(t)$, where $\operatorname{cas}'(t) = \frac{d}{dt} \operatorname{cas}(t)$. The properties of the cas function are:

$$\begin{aligned} \operatorname{cas}(u+v) &= \cos u \operatorname{cas} v + \sin u \operatorname{cas}' v, \\ \operatorname{cas}(u-v) &= \cos u \operatorname{cas}' v + \sin u \operatorname{cas} v, \\ \operatorname{cas} u \operatorname{cas} v &= \cos(u-v) + \sin(u+v), \\ \operatorname{cas} u + \operatorname{cas} v &= 2 \operatorname{cas} \frac{1}{2}(u+v) \cos \frac{1}{2}(u-v), \\ \operatorname{cas} u - \operatorname{cas} v &= 2 \operatorname{cas}' \frac{1}{2}(u+v) \sin \frac{1}{2}(u-v). \end{aligned}$$

Let the even and odd parts of $H(\omega)$ be denoted by $E(\omega)$ and $O(\omega)$, respectively. Then $E(-\omega) = E(\omega)$ and $O(-\omega) = -O(\omega)$, and we have

$$\begin{aligned} E(\omega) &= \frac{H(\omega) + H(-\omega)}{2} = \int_{-\infty}^{\infty} f(t) \cos(2\pi\omega t) dt, \\ O(\omega) &= \frac{H(\omega) - H(-\omega)}{2} = \int_{-\infty}^{\infty} f(t) \sin(2\pi\omega t) dt, \end{aligned}$$

and

$$E(\omega) - i O(\omega) = \int_{-\infty}^{\infty} f(t) e^{-2\pi i \omega t} dt.$$

Comparing with the Fourier transform $F(\omega)$, we find that $\Re\{F(\omega)\} = E(\omega)$, $\Im\{F(\omega)\} = -O(\omega)$, and conversely, $H(\omega) = \Re\{F(\omega)\} - \Im\{F(\omega)\}$.

Let the asterisk $*$ denote the convolution and the pentagram \star the cross-correlation of two functions $f_1(t)$ and $f_2(t)$. Then

$$\begin{aligned} f_1(t) * f_2(t) &= \int_{-\infty}^{\infty} f_1(t-u) f_2(u) du, \\ f_1(t) \star f_2(t) &= \int_{-\infty}^{\infty} f_1(t+u) f_2(u) du. \end{aligned}$$

If one or both of the functions entering into convolution is either even or odd, then the Hartley theorem on convolution is the same as the Fourier theorem; i.e., if $f_1(t)$ is even, then $f_1(t) * f_2(t)$ has the Hartley transform $H_1(\omega)H_2(\omega)$. But if one of the functions is odd, there is a corresponding simplification, that is, if $f_1(t)$ is odd, then $f_1(t) * f_2(t)$ has the Hartley transform $H_1(\omega)H_2(-\omega)$. The theorems for the Fourier and Hartley transform are compared in [Table 6.7.1](#).

Table 6.7.1. Theorems for Fourier and Hartley Transforms.

Theorem	$f(t)$	$F(\omega)$	$H(\omega)$
Similarity	$f(t/T)$	$ T F(T\omega)$	$ T H(T\omega)$
Addition	$f_1(t) + f_2(t)$	$F_1(\omega) + F_2(\omega)$	$H_1(\omega) + H_2(\omega)$
Reversal	$f(-t)$	$F(-\omega)$	$H(-\omega)$
Shifting	$f(t - c)$	$e^{-2\pi i c \omega} F(\omega)$	$\sin(2\pi c \omega) H(-\omega) + \cos(2\pi c \omega) H(\omega)$
Modulation	$f(t) \cos(2\pi \omega_0 t)$	$\frac{1}{2} [F(\omega - \omega_0) + F(\omega + \omega_0)]$	$\frac{1}{2} [H(\omega - \omega_0) + H(\omega + \omega_0)]$
Convolution	$f_1(t) * f_2(t)$	$F_1(\omega) F_2(\omega)$	$\frac{1}{2} [H_1(\omega) H_2(\omega) - H_1(-\omega) H_2(-\omega) + H_1(\omega) H_2(-\omega) + H_1(-\omega) H_2(\omega)]$
Autocorrelation	$f(t) \star f(t)$	$ F(\omega) ^2$	$\frac{1}{2} \{[H(\omega)]^2 + [H(-\omega)]^2\}$
Product	$f_1(t) f_2(t)$	$F_1(\omega) * F_2(\omega)$	$\frac{1}{2} [H_1(\omega) * H_2(\omega) + H_1(-\omega) * H_2(\omega) + H_1(\omega) * H_2(-\omega) - H_1(-\omega) * H_2(-\omega)]$
Derivative	$f'(t)$	$2\pi i \omega F(\omega)$	$-2\pi \omega H(-\omega)$
2nd Derivative	$f''(t)$	$-4\pi^2 \omega^2 F(\omega)$	$-4\pi^2 \omega^2 H(\omega)$

The Fourier and Hartley transform pairs, as defined by (6.1.3a–6.1.3b) and (6.7.1a–6.7.1b), respectively, deal only with continuous variables. But since the computer data is sampled at discrete intervals of time or for a specific time interval, we need discrete definitions. Thus, the discrete Hartley transform (DHT) pairs are defined by

$$H(\omega) = N^{-1} \sum_{t=0}^{N-1} f(t) \operatorname{cas}(2\pi\omega t/N), \quad (6.7.2a)$$

$$f(t) = \sum_{\omega=0}^{N-1} H(\omega) \operatorname{cas}(2\pi\omega t/N), \quad (6.7.2b)$$

where the factor N^{-1} ensures that $H(0)$ is equal to the mean value of $f(t)$, which keeps it in harmony with the convention that the Fourier coefficient a_0 be equal to the d.c. value of a periodic waveform. This can be compared with the discrete Fourier transform (DFT) defined by (6.6.2). In fact, the factor N^{-1} is borrowed from DFT practice where $F(0)$ is the d.c. value of $f(t)$; otherwise the DHT transform becomes asymmetric. Thus, the problem of computation of the DHT is analogous to that of DFT, which involves N^2 arithmetic operations to compute the DHT of N -element data. As we know, the DFT uses a permutation process to bisect the data until data pairs are reached. Then computing the Fourier transform of such data pairs becomes very rapid. The basic idea behind this permutation process in the DFT is that it is faster to split the data into pairs, compute the transform of the pairs, and recombine them to recover the entire transform rather than to compute the transform of the entire data set. Bracewell (1983) showed that precisely the same technique can be used with the DHT. The theorems for the operation of discrete Fourier and Hartley transforms are compared in Table 6.7.2.

The Hartley transform of a data pair, say, a and b , is $\frac{1}{2}(a+b, a-b)$, and computation of such pairs is very simple. Also, these two-element sequences (pairs) can be superimposed to compute the Hartley transform of the input data set. However, for this purpose we need a formula that expresses a complete DHT in terms of its half-length subsequences. The general decomposition formula for bisecting the data is (Bracewell 1983)

$$H(\omega) = H_1(\omega) + H_2(\omega) \cos(2\pi\omega/N_s) + H_2(N_s - \omega) \sin(2\pi\omega/N_s), \quad (6.7.3)$$

where N_s is the number of elements in the half-length sequence; thus, $N_s = N/2$ for a data set of N elements. Formula (6.7.3) can be compared with the corresponding formula for the DFT which is $F(\omega) = F_1(\omega) + F_2(\omega) e^{2\pi i\omega/N_s}$ (see the butterfly diagram in §6.6). The butterfly diagram of the DHT for an 8-element data set is presented in Fig. 6.7.1, where the indices in the first column of the cells show the effects of the permutation on the data elements; the next three columns represent the data elements as superimposed by the decomposition formula for the butterfly computation. These cells show the three indexes of the elements. The effects of

Table 6.7.2. Theorems for Operations of Discrete Fourier and Hartley Transforms.

Theorem	Function $f(\tau)$	DFT $F(\nu)$	DHT $H(\nu)$
Reversal	$f(-\tau)$	$F(-\nu)$	$H(-\nu)$
Addition	$f_1(\tau) + f_2(\tau)$	$F_1(\nu) + F_2(\nu)$	$H_1(\nu) + H_2(\nu)$
Shifting	$f(\tau - a)$	$e^{-2\pi i a \nu / N} F(\nu)$	$\cos(2\pi a \nu / N) H(\nu) - \sin(2\pi a \nu / N) H(N - \nu)$
Convolution	$f_1(t) * f_2(t)$	$N F_1(\nu) F_2(\nu)$	$\frac{1}{2} N [H_1(\nu) H_2(\nu) - H_1(-\nu) H_2(-\nu) + H_1(\nu) H_2(-\nu) + H_1(-\nu) H_2(\nu)]$
Autocorrelation	$f(t) \star f(t)$	$\frac{1}{2} N F(\nu) ^2$	$N \{ [H(\nu)]^2 + [H(-\nu)]^2 \}$
Product	$f_1(t) f_2(t)$	$F_1(\nu) * F_2(\nu)$	$\frac{1}{2} N [H_1(\nu) * H_2(\nu) - H_1(-\nu) * H_2(-\nu) + H_1(\nu) * H_2(-\nu) + H_1(-\nu) * H_2(\nu)]$
Derivative	$f'(t)$	$2\pi i \nu F(\nu)$	$2\pi \nu H(-\nu)$
2nd Derivative	$f''(t)$	$-4\pi^2 \nu^2 F(\nu)$	$-4\pi^2 \nu^2 H(\nu)$

retrograde indexing for the 8-element data set is seen in indexes for the third and fourth iteration of the butterfly. The bottom row of the butterfly diagram gives the angular spacing (in radians) between the trigonometric coefficients.

The difference between the FFT and FHT is as follows: In FFT the elements multiplied by the trigonometric coefficients involve terms only in $F(\omega)$, but in the FHT both $H(\omega)$ and $H(N_s - \omega)$ have sine coefficients; thus, the elements multiplied by the trigonometric terms are not symmetric in the FHT. Although asymmetric, the discrete transforms can be expressed as matrix operations. While the FFT matrix terms are symmetric about the leading diagonal, the corresponding terms in the FHT are asymmetric. This asymmetry introduces some computational problems because it is difficult to process asymmetrical matrices. It leads to *retrograde indexing* which occurs when we use an independent variable as an index for the elements multiplied by the sine coefficients, thereby decreasing this index while increasing other indexes.

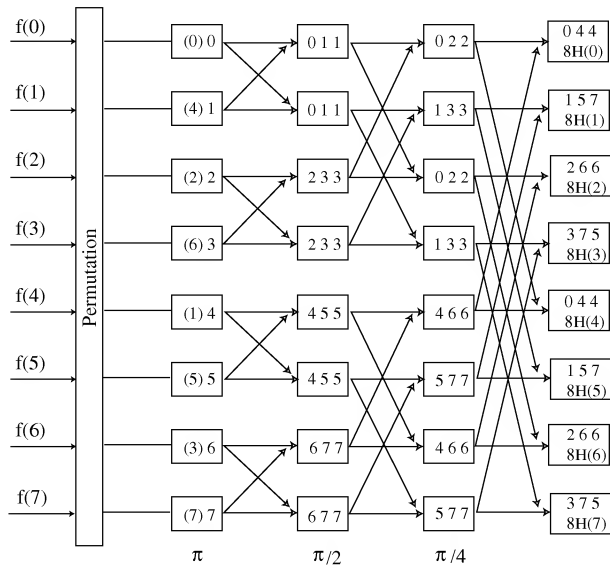


Fig. 6.7.1. Butterfly Diagram for the HFT.

The inverse Hartley transform can be obtained by applying the FHT algorithm again to its own output, which regenerates the input data. This means that we can use the same computer program to compute the transform and its inverse. But there is a slight asymmetry between the FHT and its inverse obtained by this method. In the case of the time-to-frequency transform, to obtain the discrete Hartley transform, we must scale the result of the butterfly computation by dividing the output of the butterfly by N , where N denotes the number of elements in the input data set. However, this is not needed for frequency-to-time transform; thus, the butterfly computation is itself the inverse transform. All we need is to attach a code to control whether the scaling is applied during a conversion.

6.7.1. Comparison of the FFT and FHT Algorithms. This comparison deals with the following issues.

1. The FHT algorithm can be used in many applications where FFT is applicable.

2. The Fourier transform itself can be obtained from the Hartley transform, and it is faster to generate the Fourier transform and power spectrum with the FHT than with the FFT, because computation of the butterfly using real quantities rather than the complex ones needs fewer floating-point operations.

3. The real and imaginary parts of the (complex) FFT can then be obtained from the FHT at the end of the computation by using the formulas

$$\Re\{F(\omega)\} = H(\omega) + H(N - \omega), \quad \Im\{F(\omega)\} = H(\omega) - H(N - \omega), \quad (6.7.4)$$

where N denotes the number of elements in the data set.

4. The power spectrum P_s can be computed directly from the Hartley transform by using the formula

$$P_s(\omega) = \frac{1}{2} [H(\omega)^2 + H(N - \omega)^2]. \quad (6.7.5)$$

5. The formula for the convolution of a pair of functions is almost identical in Hartley or Fourier transform (see formula (6.1.6) for the Fourier transform). The convolution of a pair of functions for the Hartley transform is defined by

$$f_1(t) \star f_2(t) = H_1(\omega) H_{2e}(\omega) + H_1(-\omega) H_{2o}(\omega), \quad (6.7.6)$$

where the subscript ‘ e ’ and ‘ o ’ denote the even and odd parts of the Hartley transform, such that if one of the functions being convoluted is either even or odd, the form of the convolution (6.7.6) reduces to the simpler formula

$$f_1(t) \star f_2(t) = H_1(\omega) H_2(\omega), \quad (6.7.7)$$

which is similar to (6.1.6). Since in practical applications many convolution functions are even, e.g., the Gaussian function used in image processing, we can use formula (6.7.7) with computational advantage.

6. As in the case of FFT, the FHT algorithm will produce an erroneous frequency function if the data set to be transformed does not approach zero smoothly at both endpoints of the range. This phenomenon is known as the *spectral leakage*, which can be reduced by multiplying the data set to be transformed by a suitable *window function* $W(n)$ prior to computing the transform. Such window functions are discussed in Stigall et al. (1982) in their effect on the power spectrum. Some window functions are described below. Additional information is available in Harris (1978) and Nutall (1980).

(i) TRIANGULAR WINDOW is defined by

$$W(n) = \frac{2(n + 0.5)}{n},$$

$$W(N - n - 1) = W(n), \quad n = 0, 1, \dots, N/2; \quad (6.7.8a)$$

it is of a low quality, but very fast, and is used to filter noise from telemetry signals in real time.

(ii) HANNING WINDOW is defined by

$$W(n) = 0.5 \left(1 - \cos \frac{2\pi(n+0.5)}{N} \right), \quad n = 0, 1, \dots, N-1. \quad (6.7.8b)$$

(iii) HAMMING WINDOW is defined by

$$W(n) = 0.54 - 0.46 \left(1 - \cos \frac{2\pi(n+0.5)}{N} \right), \quad n = 0, 1, \dots, N-1. \quad (6.7.8c)$$

(iv) BLACKMAN WINDOW is for data sets where the Hanning/Hamming windows are not suitable. It is defined by

$$W(n) = 0.42 - 0.4 \cos \frac{2\pi(n+0.5)}{N-1}, \quad n = 0, 1, \dots, N-1. \quad (6.7.8d)$$

6.7.2. FHT2D Program. The computer code `ht.f90` uses the ‘cas’ function to compute the discrete Hartley transform y of a given data set x . A driver program, `ht2d.f90`, initializes the test data set, computes the Hartley coefficients, the inverse of the coefficients (which should be the original data), and prints the results. A second code for computing Hartley transforms is `hartley2d.f90` with its driver program `xfht.f90`. The `hartley2d.f90` program does not use the ‘cas’ function approach and produces slightly different results than those obtained by `ht.f90`. The corresponding MATLAB codes are `fht.m` and `fht2d.m`, and the Mathematica code is `fht2d.nb`. All these codes are available on the CD-R.

7

Inversion of Laplace Transforms

The inversion of the Laplace transform on the real line is well known to be an ill-posed problem, since it basically deals with solving a Fredholm integral equation of the first kind (see [Chapter 9](#)). In view of this ill-posedness, there are different Laplace inversion methods, some of which, as expected, give better results for certain classes of transforms and not for all transforms. In this chapter we present various approximation formulas for the indicial function $f(t)$ and indicate where a particular method converges and where it fails numerically.

7.1. Use of Orthogonal Polynomials

The Laplace transform pair is defined as

$$\mathcal{L}\{f(t)\} \equiv \bar{f}(s) = \int_0^{\infty} f(t)e^{-st} dt, \quad \Re\{s\} > c, \quad (7.1.1)$$

$$\mathcal{L}^{-1}\{\bar{f}(s)\} \equiv f(t) = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} \bar{f}(s) e^{st} ds, \quad (7.1.2)$$

if the function $\bar{f}(s)$ exists, such that all singularities of $\bar{f}(s)$ are situated to the left of $\Re\{s\} > c$. The integral (7.1.2) is known as the Bromwich integral (also as Mellin integral), and the function $f(t)$ is sometimes called the indicial function. The Laplace transform $\bar{f}(s)$ exists for $s > c$, if the function $f(t)$ is piecewise continuous for $t > 0$ in every finite closed interval $0 \leq t \leq T$ ($T > 0$), and if $f(t)$ is of exponential order α , i.e., there exist α , $M > 0$, and $t_0 > 0$ such that $e^{-\alpha t} |f(t)| < M$ for $t > t_0$. The inversion of Laplace transforms can be regarded as a special case of

integral equations of the first kind on the interval $(0, \infty)$, where the free term is $\bar{f}(s)$ whose inverse Laplace transform is an unknown function $f(t)$ for $0 < t < \infty$. It is also obvious from the effect of a small-amplitude perturbation, which yields $\mathcal{L}^{-1}\{\bar{f}(s) + (s - 1 - ib)^{-1}\} = f(t) + e^{(1+ib)t}$, that as $b \rightarrow +\infty$, the perturbation $(s - 1 - ib)^{-1}$ tends uniformly to zero on the real line, but the corresponding term on the right becomes unbounded. Also, the inversion problem is ill-posed (see [Chapter 9](#)), which makes it very interesting. We will present different numerical methods for computing the function $f(t)$.

Some of the earliest theoretical results on the inversion problem are those by Post (1930), Widder (1935), Bateman (1936), and Boas and Widder (1940). These results deal with the integral (7.1.2). Thus, Post and Widder prove that

$$f(t) = \lim_{k \rightarrow \infty} \frac{t^{k-1}}{k! (k-2)!} \int_0^\infty \frac{\partial^k}{\partial u^k} [u^{2k-1} e^{-iu}] \bar{f}(u) du, \quad (7.1.3)$$

whereas Boas and Widder show that if the integral (7.1.2) converges for $s > c_0$, then for each $c > c_0$

$$f(t) = \lim_{k \rightarrow \infty} e^{ct} t^{k-1} \int_0^\infty Q_k(t, u) \bar{f}(u+c) du, \quad (7.1.4)$$

where $Q_k(t, u) = c_k \frac{\partial^k}{\partial u^k} [u^{2k-1} e^{-iu}]$, with $c_1 = 1$, and $c_k = \frac{1}{k! (k-2)!}$ for $k \geq 2$. Formula (7.1.4) holds for $f \in L_1(0, \infty)$. Recently, Byun and Saitoh (1993), assuming that $f \in L_2(0, \infty)$, obtain the representation

$$f(t) = \int_0^\infty \bar{f}(s) e^{-st} p_N(st) ds, \quad N = 0, 1, 2, \dots,$$

where $p_N(x)$ are the polynomials defined by

$$\begin{aligned} p_N(x) = & \sum_{0 \leq \nu \leq n \leq N} \frac{(-1)^{\nu+1} (2n)!}{(n+1)! \nu! (n-\nu)! (n+\nu)!} x^{n+\nu} \\ & \times \left\{ \frac{2n+1}{n+\nu+1} x^2 - \left(\frac{2n+1}{n+\nu+1} + 3n+1 \right) x + n(n+\nu+1) \right\}. \end{aligned} \quad (7.1.5)$$

It is proved that the sequence $\{f_N(t)\}_{N=0}^\infty$ converges to $f(t)$ in the sense that $\lim_{N \rightarrow \infty} \int_0^\infty |f(t) - f_N(t)|^2 dt = 0$. The representation (7.1.5) is generalized by Byun and Saitoh to functions $f \in L_{2,q}$, $q > 0$, which is the class of all square integrable functions with respect to the measure $t^{1-2q} dt$ on the half-axis $(0, \infty)$, and they prove that

$$f(t) = s - \lim_{N \rightarrow \infty} \int_0^\infty \bar{f}(s) e^{-st} p_{N,q}(st) ds, \quad (7.1.6)$$

where

$$p_{N,q}(x) = \sum_{0 \leq \nu \leq n \leq N} \frac{(-1)^{\nu+1} \Gamma(2n+2q)}{\nu! (n-\nu)! \Gamma(n+2q+1) \Gamma(n+\nu+2q)} x^{n+\nu+2q-1} \\ \times \left\{ \frac{2(n+q)}{n+\nu+2q} x^2 - \left(\frac{2(n+q)}{n+\nu+2q} + 3n+2q \right) x + n(n+\nu+2q) \right\},$$

and the limit is taken in the $L_{2,q}$ space of the polynomials $p_{N,q}(x)$. Note that for $q = 1/2$ the polynomials $p_{N,1/2}$ is different from that in Boas and Widder.

Krylov and Skoblya (1977) describe the following three methods which use orthogonal polynomials. Let $p_n(x)$, $n = 0, 1, 2, \dots$, denote a system of orthogonal polynomials on $[0, 1]$ with respect to the weight $w(x)$. The related generalized Fourier series for $\phi(x)$ is

$$\phi(x) \sim \sum_{k=0}^{\infty} a_k p_k(x), \quad a_k = \int_0^1 w(x) \phi(x) p_k(x) dx. \quad (7.1.7)$$

If we take a finite sum of the n terms of the series as

$$S_n(x) = \sum_{k=0}^n a_k p_k(x),$$

then the polynomial $S_n(x) \in \mathcal{P}_n$ can be regarded as an approximation to the function $\phi(x)$. Thus, the function $\phi(x)$ can be expressed in terms of orthogonal polynomials $p_n(x)$ by $\phi(x) = \sum_{k=0}^n c_k p_k(x)$. Now, we will consider some special cases of the weight function $w(x)$.

SHIFTED JACOBI POLYNOMIALS. (§1.2.11) Denote $P_n^{*(\alpha,\beta)}(x) = \sum_{i=0}^n \alpha_i^{(n)} x^i$.

The weight function is $w(x) = x^\alpha(1-x)^\beta$, and $a_k = c_k/\sqrt{r_k}$, $k = 0, 1, \dots, n$, where

$$c_k = \sum_{i=0}^k \alpha_i^{(k)} \bar{f}(i). \quad (7.1.8)$$

$$r_k = \frac{\Gamma(k+\alpha+1) \Gamma(k+\beta+1)}{k! \Gamma(2k+\alpha+\beta+1) \Gamma(k+\alpha+\beta+1)}, \quad (7.1.9)$$

and the image function is given by

$$f(t) = \sum_{k=0}^{\infty} a_k P_k^{*(\alpha,\beta)}(x) = \sum_{k=0}^{\infty} \frac{c_k}{r_k} P_k^{*(\alpha,\beta)}(e^{-t}). \quad (7.1.10)$$

SHIFTED LEGENDRE POLYNOMIALS. (§1.2.9) $w(x) = 1$, $r_n = 1/(2n + 1)$, and

$$f(t) = \sum_{k=0}^{\infty} (2k + 1) c_k P_k^* (e^{-t}). \quad (7.1.11)$$

SHIFTED CHEBYSHEV POLYNOMIALS. (§1.2.10) For Chebyshev polynomials $T_n^*(x)$, we have $w(x) = x^{-1/2}(1 - x)^{-1/2}$, $r_n = \pi/2$ for $n \neq 0$, and $r_0 = \pi$, and

$$f(t) = \frac{1}{\pi} \left[c_0 + 2 \sum_{k=1}^{\infty} c_k T_k^* (e^{-t}) \right], \quad (7.1.12a)$$

or, in terms of the trigonometric representation of $T_n^*(x)$,

$$f\left(-2 \ln \cos \frac{\theta}{2}\right) = \frac{1}{\pi} \left[c_0 + 2 \sum_{k=1}^{\infty} c_k \cos k\theta \right]. \quad (7.1.12b)$$

For Chebyshev polynomials $U_n^*(x)$, we have $w(x) = x^{1/2}(1 - x)^{1/2}$, $r_n = \pi/8$, and

$$f(t) = \frac{8}{\pi} \sum_{k=0}^{\infty} c_k U_k^* (e^{-t}), \quad (7.1.13a)$$

or, in terms of the trigonometric representation of $U_n^*(x)$, we have

$$f\left(-2 \ln \cos \frac{\theta}{2}\right) = \frac{8}{\pi \sin \theta} \sum_{k=0}^{\infty} c_k \sin (k + 1)\theta. \quad (7.1.13b)$$

If we use the similarity and shifting properties of the Laplace transform, we find from (7.1.1) that

$$h \bar{f}(\gamma_0 + h s) = \int_0^{\infty} e^{-\gamma_0 t/h} f\left(\frac{t}{h}\right) e^{-st} dt \quad \text{for any } h > 0.$$

If we write this expression as

$$h \bar{f}(\gamma_0 + h s) = \int_0^{\infty} e^{-st} k(t) \phi(t) dt,$$

where $k(t) \phi(t) = e^{-\gamma_0 t/h} f(t/h)$, or $\phi(t) = [k(t)]^{-1} f(t/h) e^{-\gamma_0 t/h}$, set $h = \gamma_0$, and expand $f(t/h) = k(t) e^t \phi(t)$ in terms of the shifted Legendre polynomials and shifted Chebyshev polynomials of the first and second kinds, we obtain the following expressions for $f(t/h)$:

For the shifted Legendre polynomials $P_n^*(x)$, where $k(t) = e^{-t}$, we find from (7.1.11) that

$$f(t/h) = k(t) e^t \phi(t) = \phi(t) = \sum_{k=0}^{\infty} (2k + 1) c_k P_k^* (e^{-t}). \quad (7.1.14)$$

For Chebyshev polynomials $T_n^*(x)$, where $k(t) = e^{-t/2} (1 - e^{-t})^{-1/2}$, we find from (7.1.12a) and (7.1.12b) that

$$f(t/h) = k(t) e^t \phi(t) = e^{t/2} (1 - e^{-t})^{-1/2} \phi(t), \quad (7.1.15a)$$

$$\begin{aligned} f\left(-\frac{2}{h} \ln \cos \frac{\theta}{2}\right) &= \frac{2}{\sin \theta} \phi\left(-2 \ln \cos \frac{\theta}{2}\right) \\ &= \frac{2}{\pi \sin \theta} \left[c_0 + \sum_{k=1}^{\infty} c_k \cos k\theta \right]. \end{aligned} \quad (7.1.15b)$$

For Chebyshev polynomials $U_n^*(x)$, where $k(t) = e^{-3t/2} (1 - e^{-t})^{1/2}$, we find from (7.1.12a) and (7.1.12b) that

$$f(t/h) = k(t) e^t \phi(t) = e^{-t/2} (1 - e^{-t})^{-1/2} \phi(t), \quad (7.1.16a)$$

$$\begin{aligned} f\left(-\frac{2}{h} \ln \cos \frac{\theta}{2}\right) &= \frac{1}{2} \sin \theta \phi\left(-2 \ln \cos \frac{\theta}{2}\right) \\ &= \frac{4}{\pi \sin \theta} \sum_{k=0}^{\infty} c_k \sin(k+1)\theta. \end{aligned} \quad (7.1.16b)$$

These results, though theoretically robust, do not quite sit well in computation; the factor $1/\sin \theta$ creates errors in the neighborhood of $\theta = 0$. Thus, these formulas can be used if we want to evaluate $f(t)$ in the neighborhood of some nonzero value t_0 , and not the entire real axis. In this case the parameter h can be chosen so that the substitution $x = e^{-ht}$ takes the point $t = t_0$ into $x = \frac{1}{2}$, i.e., $\theta = \pi/2$. This will reduce the effect of the factor $1/\sin \theta$ to the minimum. Since the coefficients of the Jacobi, Legendre, and Chebyshev polynomials used in these formulas as well as the coefficients c_n defined by (7.1.8) increase very rapidly with increasing n , the above formulas are not very effective unless the starting values of the ‘weighted moments’ are specified with great accuracy. The next section will discuss some application of these orthogonal polynomials in computing $f(t)$ from a given $\tilde{f}(s)$.

In a survey article Davies and Martin (1979) have discussed different methods for numerically inverting the Laplace transforms. They include methods that expand $f(t)$ in exponential functions, methods based on Gaussian quadratures using the Laguerre and Chebyshev polynomials, methods based on a bilinear transformation, methods based on Fourier series, and methods based on accelerated convergence of a Fourier series. They have compared methods by Bateman (1936), Bellman, Kalaba and Lockett (1966), Cooley, Lewis and Welch (1970), Cost (1964), Crump (1976), Dubner and Abate (1968), Durbin (1974), Lanczos (1956), Papoulis (1956), Piessens (1969, 1971, 1973, 1975), Piessens and Branders (1971), Salzer (1955), Schapery (1962), Stehfest (1970), ter Haar (1951), Weeks (1966), and Widder (1934). In the

sequel we will discuss these methods and others. Davies and Martin (1979) have also presented two measures for the accuracy of the numerical solution; they are

$$L = \sqrt{\sum_{j=1}^{30} \left(f(0.5j) - \tilde{f}(0.5j) \right)^2 / 30}, \quad (7.1.17)$$

$$L_e = \sqrt{\left(\sum_{j=1}^{30} \left(f(0.5j) - \tilde{f}(0.5j) \right)^2 e^{-j/2} \right) / \left(\sum_{j=1}^{30} e^{-j/2} \right)}, \quad (7.1.18)$$

where L gives the root-mean-square deviation of analytical solution $f(t)$ and the approximate solution $\tilde{f}(t)$ for values of $t = 0.5(0.5)15$, and L_e is a similar measure weighted by the factor e^{-t} .

7.2. Interpolatory Methods

We use the following property of Laplace transforms: If $\Re\{s\} > 0$ and all singularities of $\bar{f}(s)$ are located to the right of the line $\Re\{s\} = c > 0$, and if $f(t)$ is of the exponential order α , then $\lim_{\Re\{s\} \rightarrow \infty} \bar{f}(s) \rightarrow 0$, and $\bar{f}(s) = e^{-\alpha} \phi(s)$, where $\phi(s)$ is regular and bounded in the half-plane $\Re\{s\} \geq c$. The function $\phi(s)$ can then be interpolated by a linear combination of a complete system of functions. The interpolating functions are chosen with argument s^{-1} and the interpolating points along the real axis. Let $p_k(s^{-1})$ be $n+1$ interpolating polynomials of degree n in s^{-1} , and $s = s_0, s_1, \dots, s_n$ denote the nodes situated to the right of c . Then

$$\bar{f}(s) = s^{-\alpha} \phi(s), \quad \phi(s) = \sum_{k=0}^n \frac{p_k(s^{-1})}{p_k(s_k^{-1})} \phi(s_k) + r_n(s), \quad (7.2.1)$$

where

$$p_k(s^{-1}) = \frac{\prod_{i=0}^n (s^{-1} - s_i^{-1})}{(s^{-1} - s_k^{-1})}. \quad (7.2.2)$$

Using (7.2.1) and (7.2.2) in the integral (7.1.2), we obtain

$$f(t) = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} \left[s^{-\alpha} e^{st} \sum_{k=0}^n \frac{p_k(s^{-1})}{p_k(s_k^{-1})} \phi(s_k) + r_n(s) \right] ds = A_k(t) \phi(s_k) + R_n,$$

where

$$A_k(t) = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} s^{-\alpha} \frac{p_k(s^{-1})}{p_k(s_k^{-1})} \phi(s_k) e^{st} ds,$$

$$R_n = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} s^{-\alpha} e^{st} r_n(s) ds.$$

If we set $\frac{p_k(s^{-1})}{p_k(s_k^{-1})}\phi(s_k) = \sum_{i=0}^k \beta_{ki}s^{-i}$, where β_{ki} are known constants, then

$$A_k(t) = \sum_{i=0}^k \frac{\beta_{ki}}{\Gamma(\alpha + i)} t^{\alpha+i-1}.$$

To simplify computation we choose the points s_i equally spaced with $s_i - s_{i-1} = 1$; then by translation along the real axis, we can take $s_0 = 1$. We will derive inversion formulas by using the Legendre, Chebyshev, Jacobi, and Laguerre polynomials; for properties of these polynomials, see §1.3.

7.2.1. Use of Legendre Polynomials.

7.2.1(a) Papoulis' Method. (Papoulis 1956) Let the logarithmic time scale x be defined by $e^{-\sigma t} = x$ for $\sigma > 0$. Then the time interval $[0, \infty)$ is mapped onto $(0, 1]$, $f(t) = f\left(-\frac{\ln x}{\sigma}\right) = \phi(x)$, and the inverse (7.1.1) becomes $\sigma \bar{f}(s) = \int_0^1 x^{(s/\sigma)-1} \phi(x) dx$, which yields

$$\sigma \bar{f}((2k+1)\sigma) = \int_0^1 x^{2k} \phi(x) dx.$$

We will extend the definition of $\phi(x)$ to the interval $(-1, 1)$ by defining $\phi(-x) = \phi(x)$. Then $\phi(x)$ becomes an even function and is expanded in terms of a series of Legendre polynomials of even order, i.e., $\phi(x) = \sum_{k=0}^{\infty} c_k P_{2k}(x)$. Hence,

$$f(t) = \sum_{k=0}^{\infty} c_k P_{2k}(e^{-\sigma t}), \quad (7.2.3)$$

where c_k are determined by taking the Laplace transform of $P_{2k}(e^{-\sigma t})$, which leads to

$$\bar{f}(s) = \frac{c_0}{s} + \sum_{k=0}^{\infty} \frac{(s-\sigma)(s-3\sigma)\dots[s-(2k-1)\sigma]}{s(s+2\sigma)\dots(s+2k\sigma)} c_k,$$

in which, by replacing s by $\sigma, 3\sigma, 5\sigma, \dots, (k+1)\sigma, \dots$, we obtain a system of $(k+1)$ equations

$$\begin{aligned} \sigma \bar{f}(\sigma) &= c_0, \quad \sigma \bar{f}(3\sigma) = \frac{1}{3} c_0 + \frac{2}{15} c_1, \\ \sigma \bar{f}((2k+1)\sigma) &= \frac{c_0}{2k+1} + \frac{2k c_1}{(2k+1)(2k+3)} + \dots \\ &\quad + \frac{2^k k! c_k}{(2k+1)(2k+3)\dots(4k+1)}. \end{aligned} \quad (7.2.4)$$

which can be solved to determine the coefficients c_k .

The choice of the scaling factor σ depends on the number of terms considered in the series (7.2.3). A simplification of formula (7.2.3) for the case of a six-term expansion is presented in the following form which minimizes the round-off errors:

$$\begin{aligned} f(t) = & \left(B_0 - \frac{B_1}{2} + \frac{3}{8} B_2 - \frac{5}{16} B_3 + \frac{35}{128} B_4 - \frac{81}{256} B_5 \right) \\ & + \frac{3}{2} \left(B_1 - \frac{5}{2} B_2 + \frac{35}{8} B_3 + \frac{85}{16} B_4 + \frac{935}{128} B_5 \right) e^{-2\sigma t} \\ & + \frac{35}{8} \left(B_2 - \frac{9}{2} B_3 + \frac{99}{8} B_4 - \frac{429}{16} B_5 \right) e^{-4\sigma t} \\ & + \frac{231}{16} \left(B_3 - \frac{13}{2} B_4 + \frac{195}{8} B_5 \right) e^{-6\sigma t} \\ & + \frac{6435}{128} \left(B_4 - \frac{17}{2} B_5 \right) e^{-8\sigma t} + \frac{46189}{256} B_5 e^{-10\sigma t}, \end{aligned} \quad (7.2.5)$$

where B_j are given in terms of the values of $s\bar{f}(s)$ in Table A.28; the quantities D_j in this table correspond to the data points such that $D_j = s\bar{f}(s)|_{s=(2j+1)\sigma}$ for $j = 0, 1, \dots, 5$; the values given in Table A.28 are the coefficients α_{jk} of D_j , where

$$B_j \text{ are defined by } B_j = \sum_{k=0}^5 \alpha_{jk} D_j.$$

7.2.1(b) Lanczos' Method. (Lanczos 1956) This method differs from the above method in that it uses the shifted Legendre polynomials which are orthogonal on the interval $(0, 1)$. Take $\xi = e^{-t}$ in (7.1.1). Then we get $f(t) = \int_0^1 f(-\ln \xi) \xi^{s-1} d\xi$, and

$$\bar{f}(k+1) = \int_0^1 f(-\ln \xi) \xi^k d\xi = \int_0^1 \phi(\xi) \xi^k d\xi = y_k,$$

where $\phi(s) = f(-\ln s)$. For an arbitrary polynomial

$$p_n(\xi) = \sum_{i=0}^n \alpha_n^i \xi^i = \alpha_n^0 + \alpha_n^1 \xi + \alpha_n^2 \xi^2 + \dots + \alpha_n^n \xi^n,$$

we have

$$\int_0^1 \phi(\xi) p_n(\xi) d\xi = \sum_{i=0}^n \alpha_n^i \int_0^1 \phi(\xi) \xi^i d\xi = \sum_{i=0}^n \alpha_n^i y_i = c_n,$$

where c_n are known because α_n^i and $y_i = \bar{f}(i+1)$ are known. We will express $\phi(x)$ in terms of the shifted Legendre polynomials $P_n^*(x)$ (see §1.3.2), which are defined on the interval $[0, 1]$ by :

$$\begin{aligned} \phi(x) &= \sum_{n=0}^n A_n P_n^*(x), \\ A_n &= (2n+1) \int_0^1 \phi(x) P_n^*(x) dx = (2n+1) c_n. \end{aligned}$$

Then we use the property $\phi(x) = f(-\ln x) = \sum_{n=0}^{\infty} (2n+1)c_n P_n^*(x)$, and find that the function $f(t)$, which is the inverse of $\bar{f}(s)$, is defined in terms of $P_n^*(x)$ by (7.1.11). Since the terms $2k+1$ and α_n^i are large, even a slight variation in c_n produces a large variation in the value of $f(t)$. In computing formula (7.1.10) we often need to evaluate c_n to well over 10 decimal digits, which becomes difficult when we are taking about 10 terms in this formula.

7.2.2. Delta Function Methods.

7.2.2(a) Cost's Method. A summary of some approximations to $f(t)$ is given in Cost (1964). These approximations are based on the sifting property of the Dirac delta function, namely, $\int_0^{\infty} f(t) \delta(t-t_0) dt = f(t_0)$, $t_0 > 0$. If we differentiate (7.1.1) n times under the integral sign with respect to s , we obtain

$$\frac{d^n}{ds^n} \bar{f}(s) = (-1)^n \int_0^{\infty} f(t) [t^n e^{-st}] dt, \quad (7.2.6)$$

where the function within the square brackets is called the intensity function. Since $\int_0^{\infty} t^n e^{-st} dt = \frac{n!}{s^{n+1}}$, we multiply the intensity function by $s^{n+1}/n!$ and obtain

$$\frac{s^{n+1}}{n!} t^n e^{-st} \approx \delta(t-t_0), \quad (7.2.7)$$

where t_0 is any specific time at which the delta function is not zero. Assuming that the delta function is located at the point $t = n/s$, which is the maximum of the left side of (7.2.7), we find from (7.2.7) that

$$\delta(t-n/s) \approx \frac{s^{n+1}}{n!} t^n e^{-st}. \quad (7.2.8)$$

Using Stirling's formula we have $\lim_{n \rightarrow \infty} \frac{s^{n+1}}{n!} t^n e^{-st} = \delta(t-n/s)$. Then substituting (7.2.8) into (7.2.6) we get

$$(-1)^n \frac{s^{n+1}}{n!} \frac{d^n}{ds^n} \bar{f}(s) = \int_0^{\infty} f(t) \delta(t-n/s) dt = f(t) \Big|_{t=n/s},$$

or

$$f(t) = \lim_{n \rightarrow \infty} \left[(-1)^n \frac{s^{n+1}}{n!} \frac{d^n}{ds^n} \bar{f}(s) \right]_{s=n/t}, \quad (7.2.9)$$

which is Widder's inversion formula.

7.2.2(b) Alfrey's Approximation. Alfrey (1944) uses the approximation formula

$$f(t) \approx \left[-s^2 \frac{d}{ds} \bar{f}(s) \right]_{s=1/t}, \quad (7.2.10)$$

which is the first-order ($n = 1$) approximation of formula (7.2.9). Hence, this formula has the same limitations as Widder's.

7.2.2(c) ter Haar's Formula. ter Haar (1951) uses the approximation

$$f(t) \approx [s \bar{f}(s)]_{s=1/t}, \quad (7.2.11)$$

which is derived by multiplying and then dividing the integrand in (7.1.1) by t , thus yielding

$$\bar{f}(s) = \int_0^\infty \frac{f(t)}{t} [t e^{-st}] dt.$$

Since $\int_0^\infty t e^{-st} st = 1/s^2$, the function in the square brackets resembles a delta function and we may, therefore, use the approximation $t e^{-st} \approx \delta(t - t_0)/s^2$. Thus,

$$s^2 \bar{f}(s) \approx \int_0^\infty \frac{f(t)}{t} \delta(t - t_0) dt, \quad (7.2.12)$$

where t_0 can be taken as the point at which $s^2 t e^{-st}$ has its maximum value. The approximation (7.2.10) follows from (7.2.12) by the sifting property of the delta function. Thus, ter Haar's approximation is of the same type as Widder's formula (7.2.9) for $n = 1$, although the indicial functions in (7.2.9) and (7.2.12) differ by a factor of $1/t$, which results in somewhat different approximations in these two cases.

7.2.2(d) Schapery's Approximation. Schapery (1962) uses a different location of the delta function, which is taken at the centroid of the intensity function in the $\log t$ scale at the point $st \approx 0.5$. Thus, this approximation is given by

$$f(t) = [s \bar{f}(s)]_{s=0.5/t}. \quad (7.2.13)$$

This method is limited to problems where $s\bar{f}(s)$ is only a linear function of $\log s$.

7.2.2(e) Least Squares Method. First proposed by Schapery (1961) and then described by Cost (1964), this method deals with the time-dependent initial and boundary value problems which have solutions of the form $f(t) = C_1 + C_2 t + \theta(t)$, where C_1 and C_2 are constants and $\theta(t)$ is the transient component of the solution defined by $\theta(t) = \int_0^\infty H(\tau) e^{-t/\tau} d\tau$, where $H(\tau)$ is a special function, which is taken as a series of delta functions such as $H(\tau) = \sum_{i=1}^m h_i (\tau - \tau_i)$. Then the function $\theta(t) = \sum_{i=1}^m h_i e^{-t/\tau_i}$ can be approximated as $\theta(t) \approx \theta^*(t) = \sum_{i=1}^m g_i e^{-t/\alpha_i}$, where g_i and α_i are constants to be determined by minimizing the mean square error E^2 between $\theta(t)$ and $\theta^*(t)$ defined by $E^2 = \int_0^\infty [\theta(t) - \theta^*(t)]^2 dt = 0$, for $i = 0, 1, \dots, m$. This minimizing process yields

$$\frac{\partial E^2}{\partial g_i} = \int_0^\infty 2 [\theta(t) - \theta^*(t)] e^{-t/\alpha_i} dt = 0, \quad i = 1, 2, \dots, m,$$

or

$$\int_0^\infty \theta(t) e^{-t/\alpha_i} dt = \int_0^\infty \theta^*(t) e^{-t/\alpha_i} dt, \quad i = 1, 2, \dots, m.$$

This mean square error will have a minimum only if the Laplace transform of the approximation is equal to that of the exact function at least at the m points $s = 1/\alpha_i$, $i = 1, \dots, m$. This provides m relations between the Laplace transform of $\theta(t)$ and that of $\theta^*(t)$, each evaluated at $s = 1/\alpha_i$, i.e.,

$$\bar{\theta}(s) \Big|_{s=1/\alpha_i} = \bar{\theta}^*(s) \Big|_{s=1/\alpha_i}, \quad i = 1, 2, \dots, m,$$

which reduces to the system of equations

$$\bar{\theta}(s) \Big|_{s=1/\alpha_i} = \sum_{j=1}^m \frac{g_j}{1/\alpha_i + 1/\alpha_j}, \quad i = 1, 2, \dots, m.$$

These equations can be solved to determine g_i in terms of the values of $\bar{\theta}(s)$ at the points $s = 1/\alpha_i$. Finally the constants C_1 and C_2 are determined from the initial and boundary conditions.

7.2.3. Use of Chebyshev Polynomials.

7.2.3(a) Lanczos' Method. (Lanczos 1956) First normalize $f(t)$ such that $f(0) = 0$, as done in §7.1.4(a) in the case of the Laguerre polynomials. We denote the normalized function by $f(t)$, set $\xi = e^{-t}$ in the inverse (7.1.1), and obtain

$$\bar{f}(s) = \int_0^1 f(-\ln \xi) \xi^{s-1} d\xi = \int_0^1 \phi(\xi) \xi^{s-1} d\xi,$$

in which substituting $\xi = (1 + \cos \theta)/2$, we get

$$f(-\ln \xi) = \phi(\xi) = \phi((1 + \cos \theta)/2) = \psi(\theta).$$

Since $\psi(0) = 0$ and $\theta = \pi$ corresponds to $t \rightarrow \infty$, we have $\psi(\pi) = 0$. Thus, $\psi(\theta)$ can be expanded in terms of $\sin k\theta$ as

$$\psi(\theta) = \frac{4}{\pi} \sum_{k=1}^{\infty} b_k \sin k\theta, \quad b_k = \frac{1}{2} \int_0^\pi \psi(\theta) \sin k\theta d\theta. \quad (7.2.14)$$

If we transform θ back to ξ , then the coefficients b_k in (7.2.14) can be expressed as

$$b_k = \frac{1}{2} \int_0^\pi \psi(\theta) \sin k\theta d\theta = \int_0^1 \phi(\xi) \frac{\sin k\theta}{\sin \theta} d\xi = \int_0^1 \phi(\xi) U_{k-1}(\xi) d\xi,$$

where $U_{k-1}(\xi)$ is the Chebyshev polynomial of the second kind and order $k-1$. If $U_k(\xi) = \sum_{i=0}^k \alpha_i \xi^i$, then

$$\begin{aligned} b_k &= \int_0^1 \phi(\xi) U_{k-1}(\xi) d\xi = \int_0^1 \phi(\xi) \sum_{i=0}^{k-1} \alpha_i \xi^i d\xi \\ &= \sum_{i=0}^{k-1} \alpha_i \int_0^1 \phi(\xi) \xi^i d\xi = \sum_{i=0}^{k-1} \alpha_i \bar{f}(i+1). \end{aligned}$$

Thus, b_k can be determined since α_i and $\bar{f}(i+1)$ are known.

7.2.3(b) Papoulis' Method. (Papoulis 1956) also uses Chebyshev polynomials. If we set $x = e^{-\sigma t} = \cos \theta$, $\sigma > 0$, then the interval $(0, \infty)$ transforms into $(0, \pi/2)$, and $f(t)$ becomes $f\left(-\frac{\ln \cos \theta}{\sigma}\right)$, which gives

$$\sigma \bar{f}(s) = \int_0^{\pi/2} (\cos \theta)^{(s/\sigma)-1} \sin[\theta f(\theta)] d\theta,$$

and with $s = (2k+1)\theta$, $k = 0, 1, 2, \dots$, we obtain

$$\sigma \bar{f}((2k+1)\theta) = \int_0^{\pi/2} (\cos \theta)^{2k} \sin[\theta f(\theta)] d\theta.$$

Without loss of generality, we assume that $f(0) = 0$; if not, then subtract a constant from $f(\theta)$, if necessary. The function $f(\theta)$ is expanded in the interval $(0, \pi/2)$ into an odd-sine series

$$f(\theta) = \sum_{k=0}^{\infty} C_k \sin(2k+1)\theta, \quad (7.2.15)$$

where the coefficients C_k are determined by solving the system

$$\begin{aligned} \frac{4}{\pi} \sigma \bar{f}(\sigma) &= C_0, \\ 2^2 \frac{4}{\pi} \sigma \bar{f}(3\sigma) &= C_0 + C_1, \\ \dots \quad \dots \quad \dots \quad \dots \quad \dots, \\ 2^{2n} \frac{4}{\pi} \sigma \bar{f}((2n+1)\sigma) &= \left[\binom{2n}{n} - \binom{2n}{2n-1} \right] C_0 \\ &\quad + \left[\binom{2n}{k} - \binom{2n}{k-1} \right] C_{n-k} + \dots + C_n, \end{aligned} \quad (7.2.16)$$

or recursively by

$$\frac{\pi}{4} C_n = \sigma 2^{2n} \frac{4}{\pi} \bar{f}((2n+1)\sigma) - \sum_{j=0}^{n-1} \left[\binom{2n}{n-j} - \binom{2n}{n-j-1} \right] C_j. \quad (7.2.17)$$

The values of the coefficients C_n on the right side of (7.2.16), computed for $n = 0, 1, \dots, 10$, are given in [Table A.29](#).

Once the coefficients C_k are determined, the function $f(\theta)$ can be computed from (7.2.15) by using the approximation

$$f_N(\theta) = \sum_{k=0}^N c_k \sin(2k+1)\theta,$$

since $f_N(\theta) \rightarrow f(\theta)$ as $N \rightarrow \infty$. This approximation is well known from the theory of Fourier series. Since $\frac{\sin(n+1)\theta}{\sin \theta} = U_n(x)$, $\cos \theta = x$ (see §1.3), where $U_n(x)$ are the Chebyshev polynomials of the second kind, and $\sin \theta = (1 - e^{-2i\sigma})^{1/2}$, we find from (7.2.15) that

$$f(t) = (1 - e^{-2i\sigma})^{1/2} \sum_{k=0}^{\infty} C_k U_{2k}(e^{-\sigma t}). \quad (7.2.18)$$

EXAMPLE 7.2.1. (Papoulis 1956) (a) $\bar{f}(s) = \frac{4}{\pi} \frac{1}{(s+0.2)^2 + 1}$, with $\sigma = 0.2$,

which has the exact solution $f(t) = \frac{\pi}{4} e^{-0.2t} \sin t$.

(b) $\bar{f}(s) = \frac{\pi}{4} \frac{1}{\sqrt{s^2 + 1}}$, $\sigma = 0.2$, which has the exact solution $f(t) = \frac{\pi}{4} J_0(t)$.

Since $f(0) \neq 0$, the function $f(\theta)$ is discontinuous at $\theta = 0$, and $f_N(\theta)$ exhibits the Gibbs phenomenon. The coefficients C_k for both examples are given in [Table 7.2.1\(a\)](#). The values of $f_N(\theta)$ computed for $\theta = 0 (\pi/36) \pi/2$ are presented in [Table 7.2.1\(b\)](#).

Other authors have used different orthogonal polynomials; e.g., Shohat (1940) uses the Laguerre polynomials; Salzer (1955) uses the generalized Bessel polynomials discovered by Krall and Frink (1949); Piessens (1969b) improves upon Salzer's work and gives a new quadrature formula for the inversion of the Laplace transform; Piessens (1971) also develops another quadrature formula using the generalized Bessel polynomials. These investigations are for a class of functions $\bar{f}(s)$ that can be approximated by polynomials in $1/s$. Luke (1968) in his review of the book by Bellman et al. (1966) suggests the use of the shifted Jacobi polynomials to compute inverse Laplace transforms. But only Piessens (1972) develops the details of such an approach, achieving better accuracy than previous methods.

Table 7.2.1(a). Values of C_n .

Example 7.2.1(a)		Example 7.2.1(b)
k	$C_k \times 10^4$	$C_k \times 10^4$
0	1724	1961
1	3154	4899
2	205	4009
3	-2075	460
4	380	633
5	530	1762
6	-754	166
7	474	862
8	-193	718
9	-40	199
10	58	982

Table 7.2.1(b). Values of $f_N(\theta)$.

Example 7.2.1(a)		Example 7.2.1(b)
θ	$f_N(\theta) \times 10^4$	$f_N(\theta) \times 10^4$
$\pi/36$	398	8133
$\pi/18$	432	8739
$\pi/12$	1158	6958
$\pi/9$	2511	7787
$5\pi/36$	3362	7896
$\pi/6$	4215	6363
$7\pi/36$	5571	5977
$2\pi/9$	6029	5241
$\pi/4$	5181	2612
$5\pi/18$	4048	615
$11\pi/36$	1944	-834
$\pi/3$	-1502	-3208
$13\pi/36$	-3272	-3190
$7\pi/18$	-1590	286
$5\pi/12$	570	1748
$4\pi/9$	694	-11
$17\pi/36$	-33	-312

7.2.4. Use of Jacobi Polynomials.

7.2.4(a) Piessens' Method. (Piessens 1972) Assume that $\bar{f}(s)$ can be represented as

$$\bar{f}(s) = s^{-a} \sum_{k=0}^{\infty} c_k P_k^{(\alpha, \beta)}(1 - bs^{-1}), \quad (7.2.19)$$

where $P_k^{(\alpha, \beta)}(\cdot)$ denotes the Jacobi polynomials of degree k , and a , α , β and b are free parameters; their choice will be discussed later. The coefficients c_k are given by

$$c_k = \frac{1}{h_k} \int_{-1}^1 (1-u)^\alpha (1+u)^\beta P_k^{(\alpha, \beta)}(u) \psi(u) du,$$

where

$$h_k = \int_{-1}^1 (1-u)^\alpha (1+u)^\beta [P_k^{(\alpha, \beta)}(u)]^2 du,$$

$$\psi(u) = \left(\frac{b}{1-u} \right)^a \bar{f}\left(\frac{b}{1-u} \right).$$

Inverting the series (7.2.19) term-by-term, we find that

$$f(t) = \frac{t^{a-1}}{\Gamma(a)} \sum_{k=0}^{\infty} c_k \frac{(\alpha+1)_k}{k!} \phi_k\left(\frac{bt}{2}\right),$$

where $(\alpha+1)_k$ is the Pochhammer's symbol, $(\alpha+1)_0 = 1$, and $\phi_k(x)$ is a polynomial of degree k defined by

$$\phi_k(x) = {}_2F_2 \left[\begin{matrix} -k, & k + \alpha + \beta + 1 \\ \alpha + 1, & a \end{matrix} ; x \right].$$

To evaluate numerical values of c_k , we note that if the series (7.2.19) is truncated after $M+1$ terms, we obtain

$$f(t) \approx \frac{t^{a-1}}{\Gamma(a)} \sum_{k=0}^M \frac{(2k + \alpha + \beta + 1) \Gamma(k + \alpha + \beta + 1)}{2^{\alpha+\beta+1} \Gamma(\alpha+1) \Gamma(k + \beta + 1)} \phi_k\left(\frac{bt}{2}\right) \sum_{j=1}^N V_j P_k^{(\alpha, \beta)}(u_j), \quad (7.2.20)$$

where N is the order of the Gauss-Jacobi quadrature formula (see §4.3.1), u_j are the nodes and $V_j = w_j \psi(u_j)$ the weights, w_j being the weights of the Gauss-Jacobi quadrature. In the special case when $\alpha = \beta = -1/2$, formula (7.2.20) becomes

$$f(t) \approx \frac{t^{a-1}}{\Gamma(a)} \sum_{k=0}^M c_k \phi_k\left(\frac{bt}{2}\right), \quad (7.2.21)$$

where

$$\phi_k(x) = {}_2F_2 \left[\begin{matrix} -k, & k \\ \frac{1}{2}, & a \end{matrix}; x \right],$$

and the coefficients c_k are obtained by using Clenshaw's method for the computation of Chebyshev coefficients as

$$c_k \approx \frac{2}{N} \sum_{m=0}^N {}''\psi \left(\cos \frac{m\pi}{N} \right) \cos \left(\frac{mk\pi}{N} \right) \quad (7.2.22)$$

or

$$c_k \approx \frac{2}{N+1} \sum_{m=0}^N {}''\psi \left(\cos \frac{(2m+1)\pi}{2(N+1)} \right) \cos \left(\frac{(2m+1)k\pi}{2(N+1)} \right), \quad k \leq N. \quad (7.2.23)$$

In formula (7.2.22) we need the value of $\lim_{s \rightarrow \infty} s\bar{f}(s)$. If this limit is not known, we use formula (7.2.23).

The polynomials $\phi_k(x)$ in formula (7.2.21) become very large as k increases, and they have alternating signs. For example, some of these polynomials are

$$\begin{aligned} \phi_0(x) &= 1, \\ \phi_1(x) &= 1 - \frac{2}{a}x, \\ \phi_2(x) &= 1 - \frac{8}{a}x + \frac{8}{a(a+1)}x^2, \\ \phi_3(x) &= 1 - \frac{18}{a}x + \frac{48}{a(a+1)}x^2 - \frac{32}{a(a+1)(a+2)}x^3, \\ \phi_4(x) &= 1 - \frac{32}{a}x + \frac{160}{a(a+1)}x^2 - \frac{256}{a(a+1)(a+2)}x^3 \\ &\quad + \frac{128}{a(a+1)(a+2)(a+3)}x^4. \end{aligned}$$

In general, by using Fasenmyer's technique (see [Rainville 1960](#)), $\phi_k(x)$ for formula (7.2.20) can be determined from the recurrence formula

$$\phi_k(x) = (A + Bx)\phi_{k-1}(x) + (C + Dx)\phi_{k-2}(x) + E\phi_{k-3}(x), \quad k \geq 3,$$

where

$$\begin{aligned} A &= \frac{(2n + \alpha + \beta)(2n + \alpha + \beta - 1)(a + n - 1)(a + n - 2)(n - 1)}{(\alpha + n)(a + n - 1)(2n + \alpha + \beta - 3)(n + \alpha + \beta)} \\ &\quad - \frac{n(2n + \alpha + \beta - 1)}{n + \alpha + \beta}, \end{aligned}$$

$$\begin{aligned}
B &= \frac{(2n + \alpha + \beta)(2n + \alpha + \beta - 1)}{(\alpha + n)(a + n - 1)(n + \alpha + \beta)}, \\
C &= -1 - A - E, \\
D &= B \frac{n - 1}{n + \alpha + \beta - 1}, \\
E &= D \frac{(n - 2)(n + \beta - 2)(a + 1 - n - \alpha - \beta)}{(2n + \alpha + \beta - 3)(2n + \alpha + \beta - 4)}, \\
\phi_0(x) &= 1, \\
\phi_1(x) &= 1 - \frac{\alpha + \beta + 2}{a(\alpha + 1)} x, \\
\phi_2(x) &= 1 - \frac{2(\alpha + \beta + 3)}{a(\alpha + 1)} x + \frac{(\alpha + \beta + 3)(\alpha + \beta + 4)}{a(a + 1)(\alpha + 1)(\alpha + 2)} x^2.
\end{aligned}$$

The parameter a must be such that $\bar{f}(s) \rightarrow s^{-a}$ as $s \rightarrow \infty$. However, there may be functions $\bar{f}(s)$ for which such an a does not exist.

Generally it is convenient to take $\alpha = \beta = -0.5$. This choice simplifies the calculations considerably. However, these values of α and β are not suitable when the Laplace transform is known in a small interval on the real line. In that case formula (7.2.22) must be used and the value of N must be so low that it satisfies the condition $\cos \frac{\pi}{2(N+1)} \leq 1 - \frac{b}{A}$, where $[0, A]$ is the interval in which $\bar{f}(s)$ is known. This restricts the number of coefficients c_k that can be calculated. The problem can be avoided by taking α large and $\beta \approx 1$.

The value of b is related to the interval of convergence on the real line for the series in (7.2.19). The minimum value of $\Re\{s\}$ for which the series in (7.2.19) is convergent is $b/2$.

Piessens computes the polynomials $\phi_k(x)$ and gives a generating formula for these polynomials. Hypergeometric functions are available in Mathematica; for details see [piessens.nb](#) on the CD-R. Finally, the error is given by

$$E(t) \approx \frac{t^{a-1}}{\Gamma(a)} c_{M+1} \phi_{M+1} \left(\frac{bt}{2} \right). \quad (7.2.24)$$

Formulas (7.2.20) and (7.2.21) are compared with those by Salzer (1958) and Luke (1969), where Salzer approximates the Laplace transform $\bar{f}(s)$ by an interpolating function $\bar{f}(s) \approx s^{-a} Q_N(1/s)$, where $Q_n(x)$ is a polynomial of degree N ; this formula uses equally spaced interpolation points $s_k = k$. The approximating function is then inverted exactly. If N is large, this inversion loses accuracy. Luke's method is a generalization of methods of Erdélyi (1943), Lanczos (1956), Miller and Guy (1966), and is also related to the method of Bellman, Kalaba and Lockett (1966) (see §4.3.1). In this method the original function $f(t)$ is obtained as a series of shifted

Jacobi polynomials

$$f(t) \approx (1 - 2^{-\lambda t})^\alpha e^{-bt} \sum_{k=0}^N a_k P_k^{(\alpha, \beta)}(2e^{-\lambda t} - 1),$$

where α, β, λ and b are free parameters, and

$$a_k = \frac{\lambda(2k + \alpha + \beta + 1)}{\Gamma(k + \alpha + 1)} \sum_{m=0}^k (-1)^m \binom{k}{m} \frac{\Gamma(2k - m + \alpha + \beta + 1)}{\Gamma(k - m + \beta + 1)} \\ \times F(\lambda(k - m + \beta + 1) - b).$$

EXAMPLE 7.2.2 Piessens (1971) considers two examples: (i) $\bar{f}(s) = \frac{1}{\sqrt{s^2 + 1}}$, for which $f(t) = J_0(t)$, and (ii) $\bar{f}(s) = \frac{e^{-(1/s)}}{\sqrt{s}}$, for which $f(t) = \frac{\cos(2\sqrt{t})}{\sqrt{\pi t}}$, and compares the results for these two examples with those of Salzer, Luke, and the exact solution.

7.2.5. Use of Laguerre Polynomials.

7.2.5(a) Lanczos' Method. (Lanczos 1956) First, normalize both $f(t)$ and $\bar{f}(s)$ by setting $s = z + a$, and multiplying both sides of the integral (7.1.2) by e^{-at} . This leads to

$$\phi(t) \equiv f(t)e^{-at} = \frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} \bar{\phi}(z)e^{zt} dz, \quad (7.2.25)$$

where $\bar{\phi}(z) = \int_0^\infty \phi(t)e^{-zt} dt$. We assume that $\phi(0) = 0$; if it is not, we replace $\phi(t)$ by $\phi^*(t) = \phi(t) - \alpha e^{-t}$, where $\alpha = \phi^*(0) = \lim_{z \rightarrow \infty} z \bar{f}(z)$. Note that $\bar{\phi}(z)$ is analytic in the right half-plane including the imaginary axis. The entire right half-plane $\Re\{z\} \geq 0$ is mapped onto the unit circle by the transformation

$$z = \frac{1-v}{1+v} = -1 + \frac{2}{1+v}, \quad dz = -\frac{2dv}{(1+v)^2} = -\frac{(z+1)^2}{2} dv,$$

which takes the imaginary axis into the unit circle. Then Eq (7.2.25) becomes

$$\phi^*(t) = \frac{1}{2i\pi} \int_{-1}^1 \bar{\phi}\left(\frac{1-v}{1+v}\right) e^{(1-v)t/(1+v)} \frac{2}{(1+v)^2} dv.$$

Using Maclaurin's expansion, we have

$$\bar{\phi}\left(\frac{1-v}{1+v}\right) \frac{2}{(1+v)^2} = \sum_{k=0}^{\infty} c_k v^k,$$

or

$$\bar{\phi}(z) = \sum_{k=0}^{\infty} 2c_k \frac{(1-z)^k}{(1+z)^{k+2}}.$$

Let $z = 1 + z_1$. Then

$$\bar{\phi}(1 + z_1) \equiv \psi(z_1) = \sum_{k=0}^{\infty} 2c_k \frac{(-1)^k z_1^k}{(2 + z_1)^{k+2}}.$$

Note that

$$\psi(z_1) = \int_0^{\infty} \phi^*(t) e^{-(1+z_1)t} dt = \int_0^{\infty} \phi^*(t) e^{-t} e^{-z_1 t} dt.$$

Thus, the problem reduces to determine $\mathcal{L}^{-1}\{\psi(z_1)\}$, which in turn will give $\mathcal{L}^{-1}\{\psi(z)\}$ and $\mathcal{L}^{-1}\{\bar{\phi}(z)\}$.

In view of $\mathcal{L}^{-1}\left\{\frac{z_1^k}{(2+z_1)^{k+2}}\right\} = \frac{d^k}{dt^k} \left[\frac{t^{k+1}e^{-2t}}{(k+1)!}\right]$, and by the definition of the Laguerre polynomials $L_n(t) = \frac{e^t}{n!} \frac{d^n}{dt^n} (t^n e^{-t})$ (see §1.3.1), we have $\mathcal{L}\{e^{-2t} L_n(2t)\} = \frac{z_1^n}{(2+z_1)^{n+1}}$. Let $g(t) = e^{-2t} [L_k(2t) - L_{k+1}(2t)]$. Then

$$\bar{g}(z_1) = \frac{z_1^k}{(2+z_1)^{k+1}} - \frac{z_1^{k+1}}{(2+z_1)^{k+2}} = \frac{2z_1^k}{(2+z_1)^{k+2}},$$

and in terms of the original variable z , this yields

$$\begin{aligned} \mathcal{L}^{-1}\left\{\frac{2(1-z)^k}{(1+z)^{k+2}}\right\} &= (-1)^k e^{-2t} [L_k(2t) - L_{k+1}(2t)] \\ &= (-1)^k [\phi_k^*(2t) - \phi_{k+1}^*(2t)], \quad \text{where } \phi_k^*(t) = e^{-t} L_k(t). \end{aligned}$$

Hence,

$$\mathcal{L}^{-1}\{\psi(z)\} = \sum_{k=0}^{\infty} (-1)^k [\phi_k^*(2t) - \phi_{k+1}^*(2t)],$$

and the function $\phi^*(t) = \phi(t) - \alpha e^{-t} = f(t) e^{-at} - \alpha e^{-t}$ is given by

$$\phi^*(t) = \sum_{k=0}^{\infty} (-1)^k c_k [\phi_k^*(2t) - \phi_{k+1}^*(2t)]. \quad (7.2.26)$$

7.2.5(b) Papoulis' Method. (Papoulis 1956) Define $\phi_n(t) = e^{-t} L_n(t)$. Then

$$\bar{\phi}_n(s) \equiv \mathcal{L}\{\phi_n(t)\} = \int_0^{\infty} \phi_n(t) e^{-st} ds = \frac{s^n}{(s+1)^{n+1}}.$$

The derivatives of $\bar{\phi}_n(s)$ of order less than n vanish at $s = 0$. Thus,

$$\begin{aligned}\frac{d^k \bar{\phi}_n(s)}{ds^k} \Big|_{s=0} &= (-1)^k \int_0^\infty t^k \phi_n(t) e^{-st} dt \Big|_{s=0} \\ &= (-1)^k \int_0^\infty t^k \phi_n(t) dt = 0, \quad k \leq n-1.\end{aligned}$$

Let $f(t) = \sum_{k=0}^\infty c_k \phi_k(t)$. Then taking Laplace transforms on both sides, we have

$$\bar{f}(s) = \sum_{k=0}^\infty c_k \frac{s^k}{(s+1)^{k+1}} = \sum_{k=0}^\infty c_k \left[\sum_{n=0}^\infty (-1)^n \binom{n+k}{k} s^{k+n} \right]. \quad (7.2.27)$$

Also, by expanding $\bar{f}(s)$ into a power series at $s = 0$, we get

$$\bar{f}(s) = \sum_{k=0}^\infty a_k s^k. \quad (7.2.28)$$

Comparing Eqs (7.2.27) and (7.2.28) and equating equal powers of s on their right sides, we find that $a_k = \sum_{n=0}^k (-1)^{k-n} \binom{k}{k-n} c_n$, which gives $c_k = \sum_{j=0}^k \binom{k}{j} a_{k-j}$.

Since a_k are known, we can find a finite number of the coefficients c_k , which approximates $f(t)$ by $f_N(t)$ defined by

$$f_N(t) = \sum_{k=0}^N C_k \phi_k(t), \quad (7.2.29)$$

where C_k are defined by (7.2.17).

7.2.5(c) Weeks' Method. (Weeks 1966) Assume that the function $f(t)$ satisfies the following integrability conditions: (i) $\int_0^\infty e^{-ct} |f(t)| dt < \infty$, and (ii) $\int_0^\infty e^{-2ct} |f(t)|^2 dt < \infty$, whenever $c \geq c_0$. Then the integral (7.1.1) defines a function $\bar{f}(s)$ which is analytic for $\Re\{s\} > c_0$, and, by the Parseval theorem, both $f(t)$ and $\bar{f}(s)$ are related by $\int_0^\infty e^{-2ct} |f(t)|^2 dt = \frac{1}{2\pi} \int_{-i\infty}^{i\infty} |\bar{f}(c+i\omega)|^2 d\omega$. Now, define a set of orthonormal polynomials $\phi_n(x) = e^{-x/2} L_n(x)$, $n = 0, 1, 2, \dots$, where $L_n(x)$ are Laguerre polynomials, and $\phi(0) = 1$. Then a function $f(t)$ can be expressed as an infinite series of the form

$$f(t) = e^{ct} \sum_{n=0}^\infty a_n \phi_n\left(\frac{t}{T}\right), \quad a_n = \frac{1}{T} \int_0^\infty e^{-ct} f(t) \phi_n\left(\frac{t}{T}\right) dt. \quad (7.2.30)$$

Denote the partial sum of the first N terms in this series $f_N(t)$. Then $f_N(t)$ will approximate $f(t)$ if we take N sufficiently large and the decay factor c and the

scale factor $T > 0$ are chosen so as to accelerate the convergence. Also, $\bar{f}_n(s) = \int_0^\infty f_N(t) e^{-st} dt \rightarrow \bar{f}(s)$ as $N \rightarrow \infty$ (Weeks 1966). Since

$$\mathcal{L}\{e^{ct}\phi_n(t/T)\} = \mathcal{L}\{e^{ct-t/(2T)} L_n(t/T)\} = \frac{(s-c-1/(2T))^n}{(s-c+1/(2T))^{n+1}},$$

we have

$$\mathcal{L}\{f_N(t)\} = \bar{f}_N(s) = \sum_{n=0}^N a_n \frac{(s-c-1/(2T))^n}{(s-c+1/(2T))^{n+1}}.$$

Thus, in view of Parseval theorem the function $f(t) - f_N(t)$ is related to its Laplace transform $\bar{f}(s) - \bar{f}_N(s)$ by

$$\int_0^\infty e^{-2ct} |f(t) - f_N(t)|^2 dt = \frac{1}{2\pi} \int_{-\infty}^\infty |\bar{f}(c+i\eta) - \bar{f}_N(c+i\eta)|^2 d\eta,$$

for $c > c_0$. Hence, for any given $\varepsilon > 0$ there exists an integer N_ε such that

$$\frac{1}{2\pi} \int_{-\infty}^\infty |\bar{f}(c+i\eta) - \bar{f}_N(c+i\eta)|^2 d\eta < \varepsilon,$$

whenever $N > N_\varepsilon$. Let $s = c + i\eta$. Then

$$\bar{f}(c+i\eta) \approx \sum_{n=0}^N a_n \frac{(i\eta - 1/(2T))^n}{(i\eta + 1/(2T))^{n+1}}.$$

Since $\left| \frac{i\eta - 1/(2T)}{i\eta + 1/(2T)} \right| = 1$, we can define a θ such that $e^{i\theta} = \frac{i\eta - 1/(2T)}{i\eta + 1/(2T)}$, solving

which we get $\eta = \frac{1}{2T} \cot \frac{\theta}{2}$. Then

$$\frac{T}{2\pi} \int_{-\pi}^\pi \left| \left(\frac{1}{2T} + \frac{i}{2T} \cot \frac{\theta}{2} \right) \bar{f} \left(c + \frac{i}{2T} \cot \frac{\theta}{2} \right) - \sum_{n=0}^N a_n e^{in\theta} \right|^2 d\theta < \varepsilon,$$

whenever $N > N_\varepsilon$. This inequality implies that

$$\left(\frac{t}{2T} + \frac{it}{2T} \cot \frac{\theta}{2} \right) \bar{f} \left(c + \frac{it}{2T} \cot \frac{\theta}{2} \right) \approx \sum_{n=0}^N a_n e^{in\theta}. \quad (7.2.31)$$

Let us denote the real and imaginary parts of $\bar{f}(c+i\eta)$ by $\bar{f}_R(c, \eta)$ and $\bar{f}_I(c, \eta)$, respectively. Then equating the real parts on both sides of Eq (7.2.31), we obtain

$$\begin{aligned} \frac{1}{2T} \left[\bar{f}_R \left(c, \frac{1}{2T} \cot \frac{\theta}{2} \right) - \cot \frac{\theta}{2} \bar{f}_I \left(c, \frac{1}{2T} \cot \frac{\theta}{2} \right) \right] &\approx \Re \left\{ \sum_{n=0}^N a_n e^{in\theta} \right\} \\ &= \sum_{n=0}^N a_n \cos n\theta = h(\theta), \end{aligned} \quad (7.2.32)$$

where the coefficients a_n are given by

$$a_0 = \frac{1}{N+1} \sum_{j=0}^N h(\theta_j), \quad a_n = \frac{2}{N+1} \sum_{j=0}^N h(\theta_j) \cos n\theta_j, \quad n \neq 0, \quad (7.2.33)$$

$$\theta_j = \left(\frac{2j+1}{N+1} \right) \frac{\pi}{2}.$$

The interpolation formulas in Eq (7.2.33) are similar to those obtained by using Chebyshev polynomials.

Although Weeks (1966) establishes the convergence of the series in Eq (7.2.30) for all positive T and for $c > c_0$, the convergence may be faster for some specific values of T and c . Based on the behavior of Laguerre functions $L_n(x)$, Weeks conjectures that $f_N(t)$ should give a good approximation for $f(t)$ for $0 < t < t_{\max}$, where $t_{\max} < 4NT$. A satisfactory choice of T is $T = t_{\max}/N$. Theoretically, the smallest value of c to ensure the convergence of the series in Eq (7.2.30) is $\Re\{s\} = c_0$ such that the rightmost singularity of $\bar{f}(s)$ lies on the line $\Re\{s\} = c_0$. However, Weeks (1966) determines empirically that a satisfactory choice of c is

$$c = (c_0 + 1/t_{\max}) U(c_0 + 1/t_{\max}), \quad (7.2.34)$$

where $U(x)$ is the unit step function. To compute the coefficients a_n in formula (7.2.21) we must determine $h(\theta)$ at the $(N+1)$ values θ_j given in (7.2.22). Thus, we compute

$$h(\theta_j) = \frac{1}{2\pi} \bar{f}_R(c, \eta_j) - \eta_j \bar{f}_I(c, \eta_j),$$

where $\eta_j = \frac{1}{2T} \cot \frac{\theta_j}{2}$, $j = 0, 1, \dots, N$. The values of η_j are calculated recursively by the formula

$$\eta_j = \frac{\gamma \eta_{j-1} - \delta}{\eta_{j-1} + \gamma}, \quad j = 1, \dots, N,$$

where $\gamma = \frac{1}{2T} \cot \theta_0 = \frac{1}{2T} \frac{\cos \theta_0}{\sin \theta_0}$, $\delta = 1/(4T^2)$, and the starting value of η_0 is given by

$$\eta_0 = \frac{1}{2T} \cot \frac{\theta_j}{2} = \frac{1}{2T} \frac{1 + \cos \theta_0}{\sin \theta_0}.$$

Once $\cos \theta_0$ and $\sin \theta_0$ are computed, the other values of $\cos \theta_j$ and $\sin \theta_j$ are calculated for $j = 1, 2, \dots, N$, by using the recursive formulas

$$\begin{aligned} \cos \theta_j &= \alpha \cos \theta_{j-1} - \beta \sin \theta_{j-1}, \\ \sin \theta_j &= \beta \cos \theta_{j-1} + \alpha \sin \theta_{j-1}, \end{aligned}$$

where $\alpha = \cos 2\theta_0 = 2 \cos^2 \theta_0 - 1$ and $\beta = \sin 2\theta_0 = 2 \sin \theta_0 \cos \theta_0$. Next, the values of $\cos n\theta_j$ for $n = 2, 3, \dots, N$, are computed from the identity $\cos n\theta_j = 2 \cos \theta_j \cos(n-1)\theta_j - \cos(n-2)\theta_j$. This completes the evaluation of the coefficients a_n . Finally, the approximation $f_N(t)$ is computed from formula (7.2.19), where the functions $\phi_n(t)$ are obtained from the recurrence relation

$$\begin{aligned}\phi_0(x) &= e^{-x/2}, \\ \phi_1(x) &= (1-x)\phi_0(x), \\ n\phi_n(x) &= (2n-1-x)\phi_{n-1}(x) - (n-1)\phi_{n-2}(x), \quad n \geq 2.\end{aligned}$$

EXAMPLE 7.2.3. (Weeks 1960) Consider $\bar{f}(s) = 1/(s^2 + s + 1)$, with exact solution as $f(t) = \frac{2}{3}e^{-t/2} \sin \frac{3t}{2}$. Define

$$\eta_j = \frac{t}{2T} \cot \frac{\theta_j}{2} = \frac{t}{2T} \left(\frac{1 + \cos \theta_j}{\sin \theta_j} \right),$$

and use Eqs (7.2.32) and (7.2.33) and the definition of $f_N(t)$. Table 7.2.3 contains the values obtained from Weeks' algorithm for $N = 30$. For computational details see [weeks.nb](#) on the CD-R.

Table 7.2.3.

t	Exact	$f_{30}(t)$,	$f_{60}(t)$
0.0	0.0	7.88(-8)	-7.5(-10)
0.5	0.353907	0.377345	0.383849
1.0	0.403341	0.533507	0.513614
1.5	0.245024	0.525424	0.479157
2.0	0.034610	0.419280	0.358920
2.5	-0.109170	0.274110	0.214463
3.0	-0.145411	0.133243	0.086115
3.5	-0.099507	0.022128	-0.006185
4.0	-0.025210	-0.049530	-0.058397
4.5	0.031623	-0.083449	-0.076518
5.0	0.051331	-0.087942	-0.071111
5.5	0.039320	-0.073722	-0.053192
6.0	0.013679	-0.050892	-0.031747
6.5	-0.008259	-0.027239	-0.012717
7.0	-0.017710	-0.007644	0.000957
7.5	-0.015174	0.005714	0.008682
8.0	-0.006552	0.012715	0.011356
8.5	0.001736	0.014511	0.010544
9.0	0.005953	0.012805	0.007881
9.5	0.005731	0.009302	0.004699
10.0	0.002921	0.005385	0.001878

For $c = 0$, our values in the third column, and also obtained by Kythe and Puri (2002), using Weeks (1966) algorithm, matched Weeks’ values exactly; however, our values in column 1, obtained for the function $f(t)$, do not match his values. However, our values are correct: Our first negative value for $f(t)$ appears at $t = 2.5$; it is because $\sin(3t/2)|_{t=2.5}$ is negative. It appears that the second column in Table 1 of Weeks’ article was accidentally replaced by his third column, since the two columns are exactly alike. The third column in Table 7.2.3 corresponds to Weeks’ algorithm with $N = 60$, and the values are generally closer to the actual values of the function, but not sufficiently accurate. Also, if we use formula (7.2.34) to determine c , then its value for $t_{\max} = 10$ should be 0.05. If we take this value of c , the values obtained from the algorithm are worse than those obtained for $c = 0$.

EXAMPLE 7.2.4. Weeks (1966) also considers the following examples:

- (i) $\bar{f}(s) = \frac{1}{s(\sqrt{s} + 1)}$, for which $f(t) = 1 - e^t \operatorname{erfc}(\sqrt{t})$;
- (ii) $\bar{f}(s) = \frac{\pi}{4} \frac{1}{\sqrt{p^2 + 1}}$, for which $f(t) = \frac{\pi}{4} J_0(t)$;
- (iii) $\bar{f}(s) = \frac{1}{s} e^{-25s}$, for which $f(t) = U(t - 25)$. We will consider one of these examples; the others can be computed similarly.

EXAMPLE 7.2.5. Consider the above example (ii). The results are given in Table 7.2.5.

TABLE 7.2.5.

t	$f_{50}(t)$ Weeks	$f_{20}(t)$ Weeks	Exact
0.01906	0.7843	0.7811	0.7853
0.07654	0.7847	0.7871	0.7842
0.17334	0.7797	0.7804	0.7795
0.11012	0.7660	0.7621	0.7665
0.49188	0.7390	0.7352	0.7386
0.71921	0.6872	0.6865	0.6871
0.99743	0.6015	0.5983	0.6019
1.33258	0.4738	0.4679	0.4736
1.73287	0.2980	0.2967	0.2976
2.20970	0.0823	0.0836	0.0824
2.77932	−0.1390	−0.1376	−0.1386
3.46574	−0.2950	−0.2869	−0.2947

Garbow, Giunta and Lyness (1988) have modified the Weeks’ method as follows. Let $c > c_0$ and $b > 0$ be two parameters. Define $g(s) = \frac{b}{1-s} \bar{f}\left(\frac{b}{1-s} + \sigma - \frac{b}{2}\right)$,

and let a_n be the Taylor's coefficient of $g(s)$, i.e., $g(s) = \sum_{n=0}^{\infty} a_n s^n$, $|s| < r$, where r is the radius of convergence of this series, and $r \geq 1$. Then

$$f(t) = e^{ct} \sum_{n=0}^{\infty} a_n \phi_n(bt), \quad c > c_0, \quad b > 0,$$

where $\phi_n(x) = e^{-x/2} L_n(x)$. Let $\tilde{f}(t)$ be an approximation of $f(t)$ by truncating the above expansion so that

$$\tilde{f}(t) = e^{ct} \sum_{n=0}^{m-1} \tilde{a}_n \phi_n(bt),$$

where the approximation \tilde{a}_n of a_n is given by

$$\tilde{a}_n = \frac{1}{m r^k} \sum_{j=1}^m g\left(r e^{2\pi i j/m}\right) e^{-2\pi i j l/m}, \quad l = 0, 1, \dots, m-1,$$

where only $m/2 + 1$ distinct evaluations of $g(s)$ are required since $g(s^*) = g^*(s)$. Based on this algorithm, Giunta, Lyness and Murli (1988) have provided a software package, called WEEKS, for the inversion problem. This program requires the transform values at arbitrary points in the complex plane \mathcal{C} and is suitable when f has continuous derivatives of all orders; it works very efficiently when $f(t)$ is required at a number of different values of t . As a test case they consider $\bar{f}(s) = 3/(s^2 - 9)$, which has the inverse $f(t) = \sinh(3t)$. The results are given in Table 7.2.5a.

Table 7.2.5a.

t	$\tilde{f}(t)$ Computed	$f(t)$ Exact	Error
0.0	9.93991(-08)	0.0	9.9(-08)
1.0	1.00179(+01)	1.001787(+01)	9.5.5(-07)
2.0	2.01713(+02)	2.017132(+02)	-1.5(-05)
3.0	4.05154(+03)	4.051542(+03)	2.0(-03)
4.0	8.13774(+04)	8.137739(+04)	-3.9(-02)
5.0	1.63451(+06)	1.634508(+06)	-7.5(-051)

Garbow and Lyness (1990) have corrected some errors in the above WEEKS program.

7.2.5(d) Piessens' Method. (Piessens 1971) It uses the Laguerre functions as follows:

$$\bar{f}(s) = s^{-a} \sum_{k=0}^{\infty} c_k L_k(bs^{-1}),$$

which, after term-by-term inversion gives

$$f(t) = \frac{t^{a-1}}{\Gamma(a)} \sum_{k=0}^{\infty} c_k \phi_k(bt), \quad (7.2.35)$$

where

$$\phi_k(x) = {}_1F_2 \left(\begin{matrix} -k \\ 1, a \end{matrix}; x \right).$$

To compute (7.2.35) we use the recurrence formula

$$\begin{aligned} \phi_n(x) = & \left[\frac{3n^2 - 5n + 2na - a + 2}{n(a+n-1)} - \frac{x}{n(a+n-1)} \right] \phi_{n-1}(x) \\ & - \frac{(3n+a-4)(n-1)}{n(a+n-1)} \phi_{n-2}(x) - \frac{(n-1)(n-2)}{n(a+n-1)} \phi_{n-3}(x), \end{aligned}$$

with the starting values $\phi_{-2}(x) = \phi_{-1}(x) = 0$ and $\phi_0(x) = 1$. The coefficients c_k are computed by using Gauss-Laguerre quadrature rule (§4.3.8), but since (7.2.24) generally converges less rapidly, this method is useful only if the coefficients c_k are previously known analytically or computationally (§7.2.4).

Some other authors who have used Laguerre polynomials are Shohat (1940), Lyness and Giunta (1986), Garbow, Giunta, Lyness, and Murli (1988a,b,c), and Giunta, Laccetti, and Rizzardi (1988).

We will now discuss the general case. Piessens (1982) notes that convergence occurs for the class S_γ of the Laplace transforms $\bar{f}(s) = s^{-\gamma} G(s)$, where $\gamma > 0$ is known and $G(s)$ is analytic at ∞ , and also for the class $S_{\gamma,\delta}$, defined in Cope (1990), where $\bar{f}(s) = s^{-\gamma} G(s^\delta)$, where $\gamma, \delta > 0$ are known and $G(w)$ is analytic at ∞ . In problems of electrochemistry, $\delta = 0.5$ is a typical case. Thus, if $\bar{f}(s) \in S_\gamma$, where $\bar{f}(s)$ is represented by $\bar{f}(s) = \sum_{k=0}^{\infty} a_n s^{-k-\gamma}$, then $f(t) = \sum_{m=0}^{\infty} \frac{a_m}{\Gamma(m+\gamma)} t^{m+\gamma-1}$, and the series converges for all t . Using the above Piessens' method on the real line, if

$$\bar{f}(s) = \sum_{k=0}^{\infty} c_k(\sigma) s^{-\gamma} p_k\left(\frac{1-2\sigma}{s}\right), \quad \sigma \leq s < +\infty,$$

then

$$f(t) = \sum_{k=0}^{\infty} c_k(\sigma) t^{\gamma-1} \phi_k(\gamma; \sigma t), \quad (7.2.36)$$

where ϕ_k are the Jacobi polynomials on $[-1, 1]$. Cope (1990) has proved that the series (7.2.36) converges for all t . The parameter σ is left arbitrary in Piessens' method, but since $G(s)$ is analytic at ∞ and $0 < s < +\infty$, any positive value for σ can be chosen. Also, the coefficients $c_k(\sigma)$ in formula (7.2.36) tend to zero exponentially

with respect to k and this exponential rate becomes slower as σ decreases to zero. In practical implementation of formula (7.2.36) where only a partial finite sum is taken, only small values of σ should be used, because such values will tend to simplify computational problems and allow us to calculate $f(t)$ over a longer time interval $0 < t < T$. As before, the coefficients $c_k(\sigma)$ are obtained by numerical quadrature. Cope (1990) has noted that although Piessens' analysis is confined to the class S_γ and $S_{\gamma,\delta}$, computer evidence indicates that this method works well for a wider range of transforms $\tilde{f}(s)$.

7.2.5(e) Lyness and Giunta's Method. As a modification of Weeks' method, Lyness and Giunta (1986) use the approximation

$$\tilde{f}(t) = e^{ct} \sum_{n=0}^N \tilde{a}_n e^{-t/(2T)} L_n\left(\frac{t}{T}\right), \quad c > c_0, \quad (7.2.37)$$

with the error estimate

$$\begin{aligned} E &= e^{-ct} \left[\tilde{f}(t) - f(t) \right] \\ &= \sum_{n=0}^N (\tilde{a}_n - a_n) e^{-t/(2T)} L_n\left(\frac{t}{T}\right) - \sum_{n=N+1}^{\infty} a_n e^{t/(2T)} L_n\left(\frac{t}{T}\right), \end{aligned}$$

where the coefficients a_n are defined in (7.2.19), and the coefficients \tilde{a}_n are determined as follows. Consider a function

$$g(z) = \frac{1}{(1-z)T} \tilde{f}\left(\frac{1}{(1-z)T} - \frac{1}{2T} + c\right),$$

which is regular within a circle $|z| < R$, $R \geq 1$. Then

$$a_n = \frac{1}{2i\pi} \int_{C:|z|=r} \frac{g(z)}{z^{n+1}} dz = \frac{1}{2\pi r^n} \int_0^{2\pi} g(re^{i\theta}) e^{-in\theta} d\theta, \quad n \geq 0. \quad (7.2.38)$$

where C is the circular contour which includes the origin but does not contain any singularity of $g(z)$. This integral is approximated by using the m -panel trapezoidal rule, with m taken to be even. Define

$$a_n^{[m,1]}(r) = \frac{1}{r^n m} \sum_{j=1}^m g\left(re^{2i\pi j/m}\right) e^{2i\pi jn/m}.$$

Since $g(z)$ is real when z is real, we have

$$\begin{aligned} a_n^{[m,1]}(r) &= \frac{2}{r^n m} \sum_{j=1}^{m/2} \left[\Re \left\{ g\left(re^{2i\pi j/m}\right) \right\} \cos(2\pi jn/m) \right. \\ &\quad \left. + \Im \left\{ g\left(re^{2i\pi j/m}\right) \right\} \sin(2\pi jn/m) \right]. \end{aligned} \quad (7.2.39)$$

Since $g(z)$ has no singularities within the circle $|z| = r$, we have, by Cauchy's theorem,

$$\frac{1}{2i\pi} \int_{|z|=r} g(z) z^{n-1} dz = \frac{r^n}{2\pi} \int_0^{2\pi} g(r e^{i\theta}) e^{in\theta} d\theta = \begin{cases} a_0, & n = 0, \\ 0, & n > 0. \end{cases} \quad (7.2.40)$$

After dividing this result by r^{2n} and then combining with (7.2.38) by taking sum and difference, we find that

$$\begin{aligned} A_n &= \frac{1}{2i\pi} \int_{|z|=r} \frac{g(z)}{z} \left(\frac{1}{z^n} + \frac{z^n}{r^{2n}} \right) dz \\ &= \frac{2}{2\pi r^n} \int_0^{2\pi} g(r e^{i\theta}) \cos n\theta d\theta = \begin{cases} 2a_n, & n = 0, \\ a_n, & n > 0, \end{cases} \\ B_n &= \frac{1}{2i\pi} \int_{|z|=r} \frac{g(z)}{z} \left(\frac{1}{z^n} - \frac{z^n}{r^{2n}} \right) dz \\ &= \frac{2}{2\pi r^n} \int_0^{2\pi} g(r e^{i\theta}) \sin n\theta d\theta = \begin{cases} 0, & n = 0, \\ ia_n, & n > 0, \end{cases} \end{aligned}$$

Thus, $2a_n = A_n - i B_n$. Two approximations of the integral representation (7.2.40) for $n = 0, 1, \dots, m/2$ are considered: one, by the m -panel midpoint rule gives

$$\begin{aligned} A_n^{[m,0]}(r) &= \frac{2}{r^n m} \sum_{j=1}^m g\left(r e^{i\pi(2j-1)/m}\right) \cos((2j-1)\pi n/m) \\ &= \frac{4}{r^n m} \sum_{j=1}^{m/2} \Re \left\{ g\left(r e^{i\pi(2j-1)/m}\right) \right\} \cos((2j-1)\pi n/m), \end{aligned}$$

and the other, by the endpoint trapezoidal rule gives

$$\begin{aligned} A_n^{[m,1]}(r) &= \frac{2}{r^n m} \sum_{j=1}^m g\left(r e^{2i\pi j/m}\right) \cos(2\pi j n/m) \\ &= \frac{4}{r^n m} \sum_{j=1}^{m/2} \Re \left\{ g\left(r e^{2i\pi j/m}\right) \right\} \cos(2\pi j n/m). \end{aligned}$$

Weeks' method uses formula (7.2.37) with $r = 1$, $N = m/2$, and $\tilde{a}_0 = \frac{1}{2} A_0^{[m,0]}(r)$, $\tilde{a}_n = A_n^{[m,0]}(r)$ for $n = 1, 2, \dots, m/2 - 1$, and $\tilde{a}_{m/2} = \frac{1}{2} A_{m/2}^{[m,0]}(r)$. Lyness and Giunta's method uses formula (7.2.37) with $r = 1$, $N = m - 1$, and $\tilde{a}_n = A_n^{[m,1]}(r)$ for $n = 0, 1, 2, \dots, m - 1$.

7.2.5(f) de Hoog's Method. (de Hoog et al. 1982) This method is based on the computation of the Bromwich integral (7.1.2) by approximating it as

$$\tilde{f}_N(t) = \frac{e^{ct}}{T} \Re \left\{ \frac{\bar{f}(c)}{2} + \sum_{k=1}^N \bar{f}(c + ik\pi/T) e^{ik\pi t/T} \right\},$$

such that $\left| \frac{f(t) - \tilde{f}_N(t)}{\tilde{f}_N(t)} \right| \leq \varepsilon$, where ε is the preassigned tolerance. D'Amore, Laccetti and Murli (1999a) improve upon this method and use Rutishauser's QD scheme to compute $\tilde{f}_N(t)$. They use a set of 38 test functions, which are available in the file `38TestFunctions.pdf` on the CD-R.

7.3. Use of Gaussian Quadrature Rules

The following three methods are considered.

7.3.1. Bellman-Kalaba-Lockett's Method. (Bellman, Kalaba, and Lockett 1966) This method uses the Gaussian quadrature to compute inverse Laplace transforms. We set $\tau = e^{-t}$, $t = -\ln \tau$, and $dt = -d\tau/\tau$ in (7.1.1). Then, taking $f(-\log \tau) = g(\tau)$, we get

$$\bar{f}(s) = \int_0^1 \tau^{s-1} f(-\log \tau) d\tau = \sum_{k=1}^N c_k w_k \tau_k^{s-1}, \quad c_k = g(\tau_k) \quad (7.3.1)$$

Since w_k , τ_k^{s-1} , and $\bar{f}(s)$ are known, this formula reduces to a system of N equations by choosing N values for s as $s = n + 1$, $n = 0, 1, 2, \dots, N - 1$; then

$$\bar{f}(n + 1) = \sum_{k=1}^N c_k w_k \tau_k^n, \quad (7.3.2)$$

which when solved for c_k gives the values of $g(\tau)$ for the N nodes. Using these values $g(\tau)$ can be approximated by a polynomial of degree $N - 1$. However, difficulty arises in the inversion of the matrix $\{w_k \tau_k^n\}$, which is often ill-conditioned. Let the solution of the system (7.3.2) be

$$c_k = g(\tau_k) = \sum_{n=0}^{N-1} \alpha_{kn} \bar{f}(n + 1),$$

and let $y_k = w_k g(\tau_k) = w_k c_k$. Then this system reduces to

$$\sum_{k=1}^N \tau_k^{i-1} y_k = a_i = \bar{f}(i).$$

Denoting the elements of the matrix of this system by $m_{ik} = \tau_k^{i-1}$, $i = 1, 2, \dots, N$, multiplying both sides of this system by q_i , and adding them we get

$$\sum_{k=1}^N y_k \left(\sum_{i=1}^N m_{ik} q_i \right) = \sum_{i=1}^N a_i q_i, \quad (7.3.3)$$

where q_i are yet to be determined. Define $l(\tau) = \sum_{k=1}^N q_k \tau^{k-1}$; then the system (7.3.3) becomes

$$\sum_{k=1}^N y_k l(\tau_k) = \sum_{i=1}^N a_i q_i. \quad (7.3.4)$$

Now we choose q_i in such a way that only one of the unknowns y_k remains in Eq (7.3.4) and the coefficients of the other unknowns become zero. This requires that we choose N values for q_i , which we denote by q_{ij} . Then define

$$l_j(\tau) = \sum_{k=1}^N q_{kj} \tau^k,$$

and choose q_{kj} such that

$$l_j(\tau_k) = \begin{cases} 0 & \text{if } k \neq j, \\ 1 & \text{if } k = j. \end{cases}$$

We can determine such q_{kj} , because $l_j(\tau)$ is a polynomial of degree $N - 1$, and therefore it satisfies N conditions. Once q_{kj} are determined, we find from (7.3.4) that $y_i = \sum_{k=1}^N a_k q_{ki}$, or $g(\tau_i) = \sum_{k=1}^N \frac{1}{w'_i} a_k q_{ki}$.

EXAMPLE 7.3.1. $\bar{f}(s) = \frac{1}{s^2 + 1}$, $f(t) = \sin t$. We use $P_9^*(x)$, which has zeros x_i and the modified weights w'_i as given in Example 1.3.1. Then the system of equations (7.3.2) is given by

$$\begin{aligned} \bar{f}(n+1) = & (0.0406376)(0.01592)^n c_1 + (0.0903246)(0.0819845)^n c_2 \\ & + (0.1303056)(0.193314)^n c_3 + (0.1561712)(0.337874)^n c_4 \\ & + (0.1651198)(0.5)^n c_5 + (0.1561712)(0.6621265)^n c_6 \\ & + (0.1303056)(0.806686)^n c_7 + (0.0903246)(0.9180155)^n c_8 \\ & + (0.0406376)(0.98408)^n c_9 \quad \text{for } n = 0, 1, \dots, 8, \end{aligned}$$

and we obtain

$$c_i = \left\{ -0.555427, 0.531849, 1.0262, 0.867557, 0.650197, 0.392641, \right. \\ \left. 0.219162, 0.0810746, 0.018805 \right\}, \quad i = 1, 2, \dots, 9.$$

Thus, the function $f(t) = f(-\ln x) = g(x)$, $g(x_1) = c_i$ is known at the nine points x_i . Further, if we assume that

$$g(x) = \sum_{k=1}^9 B_k x^{k-1},$$

then we can obtain nine equations by letting $x = x_i$ for $i = 1, 2, \dots, 9$, and solve for B_k , which are given by

$$B_k = \{ -0.5554273121669501, 0.5318493617139866, 1.0262029177215746, \\ 0.8675569112458106, 0.6501966073073655, 0.39264073646123254, \\ 0.21916193172192688, 0.08107463934338578, 0.018805014457441416 \}.$$

Now, $f(t)$ can be approximated by

$$\begin{aligned} \tilde{f}(t) = & -0.953120649827127 + 26.85593411635183e^{-t} \\ & - 120.02973389488155e^{-2t} + 133.11599313846204e^{-3t} \\ & + 511.05194566693484e^{-4t} - 1962.8192889883146e^{-5t} \\ & + 2790.690732420141e^{-6t} - 1864.0777367913424e^{-7t} \\ & + 486.19656491268586e^{-8t}. \end{aligned}$$

Table 7.3.1 gives the values of $\sin t$ and above approximate solution $\tilde{f}(t)$. For computational details see `bellman.nb` on the CD-R. ■

Table 7.3.1

t	Exact	$\tilde{f}(t)$	Error
0.0	0.0	0.0312	3.1(−2)
0.5	0.479426	0.48193	2.5(−3)
1.0	0.841471	0.825406	1.6(−2)
1.5	0.997495	1.01933	2.1(−2)
2.0	0.909297	0.910953	1.6(−3)
10.0	−0.544021	−0.951902	7.8(−3)

EXAMPLE 7.3.2. $\bar{f}(s) = \frac{1}{s+1}$, $f(t) = e^{-t}$.

Following the steps of in Example 7.3.1, the approximation for e^{-t} corresponding to (7.2.29) is

$$\begin{aligned} \tilde{f}(t) = & -(5.400809667158862)10^{-6} + 1.000508184397117e^{-t} \\ & - 0.011280122194696447e^{-2t} + 0.09671775139664975e^{-3t} \\ & - 0.399801991834753e^{-4t} + 0.8833083132385336e^{-5t} \\ & - 1.067983373238557e^{-6t} + 0.6661710928983806e^{-7t} \\ & - 0.1676435041570735e^{-8t}. \end{aligned}$$

Table 7.3.2 gives the values of $f(t) = e^{-t}$ and the approximate values $\tilde{f}(t)$ obtained from the above approximation. For computational details, see `bellman.nb` on the CD-R. ■

Table 7.3.2

t	Exact	$\tilde{f}(t)$	Error
0	1.0	0.999991	9.0(−6)
1	0.367879	0.367883	4.0(−6)
2	0.135335	0.135332	3.0(−6)
3	0.0497871	0.0497887	1.6(−6)
4	0.0183156	0.0183163	7.0(−7)

Some improvements to this method are as follows:

7.3.2. Felts and Cook’s Method. (Felts and Cook 1969) If we make a change of variables $t = -\ln(x/T)$ in (7.1.1), we obtain

$$\bar{f}(s) = \frac{1}{T} \int_0^T \left(\frac{x}{T}\right)^{s-1} f\left(-\ln\left(\frac{x}{T}\right)\right) dx, \tag{7.3.5}$$

which can be expressed as the sum of two integrals

$$\bar{f}(s) = \frac{1}{T} \left(\int_0^{T/2} + \int_{T/2}^T \right) \left(\frac{x}{T}\right)^{s-1} f\left(-\ln\left(\frac{x}{T}\right)\right) dx \equiv I_1 + I_2.$$

We will make change of variables in I_1 and I_2 so that the interval of integration in each is changed to $[0, 1]$, which will permit use of the Gauss-Legendre quadrature formula with the shifted Legendre polynomials $P_n^*(x)$. Thus, in I_1 we set $x = Ty/2$ and in I_2 set $x = T(y + 1)/2$. Then

$$\begin{aligned} \bar{f}(s) = \frac{1}{2} \bigg[&\int_0^1 \left(\frac{y}{2}\right)^{s-1} f\left(-\ln\left(\frac{y}{2}\right)\right) dy \\ &+ \int_0^1 \left(\frac{y+1}{2}\right)^{s-1} f\left(-\ln\left(\frac{y+1}{2}\right)\right) dy \bigg]. \end{aligned} \tag{7.3.6}$$

If we apply Gauss-Legendre quadrature to each of the integrals in (7.3.6) and allow s to take $2N$ real values $s = k + 1, k = 0, 1, \dots, (2N - 1)$, then we obtain

$$\begin{aligned} \bar{f}(k + 1) \approx \frac{1}{2} \bigg\{ &\sum_{j=1}^N \left[W_j \left(\frac{y_j}{2}\right)^k\right] f\left(-\ln\left(\frac{y_j}{2}\right)\right) \\ &+ \sum_{j=1}^N \left[W_j \left(\frac{y_j + 1}{2}\right)^k\right] f\left(-\ln\left(\frac{y_j + 1}{2}\right)\right) \bigg\}, \quad k = 0, 1, \dots, (2N - 1), \end{aligned} \tag{7.3.7}$$

in which the two matrices within square brackets are to be computed.

A generalization of formula (7.3.6) from two integrals to an arbitrary number m of integrals is obtained by expressing the integral (7.3.5) as the sum of m integrals

$$\bar{f}(s) = \frac{1}{T} \sum_{i=1}^m \int_{(m-i)T}^{(m-i+1)T} \left(\frac{x}{T}\right)^{s-1} f\left(-\ln\left(\frac{x}{T}\right)\right) dx, \quad (7.3.8)$$

where the intervals of integration can be transformed to $[0, 1]$ by setting $x = \frac{T}{m}y + \frac{(m-i)T}{m}$. Then (7.3.8) becomes

$$\bar{f}(s) = \frac{1}{m} \sum_{i=1}^m \int_0^1 \left(\frac{y}{m} + \frac{m-i}{m}\right)^{s-1} f\left(-\ln\left(\frac{y}{m} + \frac{m-i}{m}\right)\right) dy. \quad (7.3.9)$$

Applying the quadrature approximation to the m integrals in (7.3.9) and letting s take on the real integral values $s = k + 1$, $k = 0, 1, \dots, (mN - 1)$, we obtain

$$\bar{f}(k+1) = \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^N [W_j (t_{ij})^k] f(-\ln(t_{ij})), \quad (7.3.10)$$

where $t_{ij} = \frac{y_j}{m} + \frac{m-i}{m}$. Formula (7.3.10) has an $(mN) \times N$ matrix which must be computed for each of the m integrals. Note that for $m = 2$ formula (7.3.10) reduces to (7.3.7).

Felts and Cook (1969) have computed tables for $\bar{f}(k+1)$ for $m = 1$ and $N = 32$, $m = 2$ and $N = 16$, and $m = 4$ and $N = 8$, and compared the results with the exact values of $\bar{f}(s)$ at the points t_{ij} for the function

$$\bar{f}(s) = \frac{a_1 s + a_0}{[(s_b)^2 + d_1^2][(s+c)^2 + d_2^2]},$$

for $a_0 = 16$, $a_1 = 32$, $b = 1$, $c = 3$, $d_1 = \sqrt{15}$, and $d_2 = \sqrt{27}$. These computed values are used in the Gauss-Legendre formula developed by Bellman, Kagiwada and Kalaba (1965), although they can be used in any one of the above Gauss-Legendre formulas, say (9.1.7), to approximate $f(t)$.

7.3.3. Piessens' Method. (Piessens 1969a) starts with summarizing the method of Bellman et al. (1966) by applying the Gauss-Legendre quadrature rule to (7.3.1), which gives

$$\bar{f}(s) \approx \sum_{i=1}^N w_i \tau_i^{s-1} f(-\ln \tau_i),$$

where τ_i is the i -th zero of the shifted Legendre polynomial $P_N^*(x)$ and w_i is the corresponding weight. If we let s assume N different values, e.g., $s = 1, 2, \dots, N$,

we obtain a system of N linear equations in N unknowns $f(-\ln \tau_i)$, $i = 1, 2, \dots, N$, which can be solved explicitly to yield

$$f(t_i) \approx \sum_{k=1}^N a_{ik}^{(N)} \bar{f}(k), \quad (7.3.11)$$

where $t_i = -\ln \tau_i$, and the coefficients $a_{ik}^{(N)}$ are tabulated by Bellman et al. (1966). The drawback with the inversion formula (7.3.11) is that it gives values of $f(t)$ in a restricted number of nonequidistant points. Piessens (1969a) has modified formula (7.3.11) by approximating $\bar{f}(s)$ by an interpolating rational function

$$\bar{f}(s) = \sum_{k=1}^N (-1)^{N-k} \frac{(k+N-1)! \prod_{m=1, m \neq k}^N (s-m)}{[(k-1)!] (N-k)! \prod_{m=0}^{N-1} (s+m)}, \quad (7.3.12)$$

which is a generalized Lagrange interpolation polynomial in the points $s = 1, 2, \dots, N$. Inverting (7.3.12) we obtain the formula

$$f(t) \approx \sum_{k=1}^N \phi_k^{(N)}(e^{-t}) \bar{f}(k), \quad (7.3.13)$$

where $\phi_k^{(N)}(x)$ is a polynomial of degree $N-1$, defined by

$$\phi_k^{(N)}(x) = \sum_{m=1}^N \frac{(-1)^{k+m-1} (N+k-1)! (N+m)! x^m}{[(k-1)!]^2 (N-k)! (m!)^2 (N-m-1)! (k+m)}. \quad (7.3.14)$$

The coefficients of $\phi_k^{(N)}(x)$ can be easily computed (see [coeffs.nb](#) on the CD-R). Piessens (1969a) has provided a table of these coefficients for $N = 3(1)7$, which is presented as [Table A.30](#). Using these values of the coefficients he computes two tables of the values of $\phi_k^{(N)}(e^{-t})$, one for $N = 6$ and $t = 0.0(0.5)7.0$, and the other for $N = 10$ and $t = 0.0(0.5)10..$

Piessens (1969c) considers the integral (7.1.2) which, after setting $st = u$ and assuming $\bar{f}(s) = u^{-\gamma} G(u)$, where γ is a parameter, yields the approximation

$$tf(t) = \frac{1}{2i\pi} \int_{L'} e^u u^{-\gamma} G(u) du \approx \sum_{k=1}^N A_k G(u_k), \quad (7.3.15)$$

where L' is the line $\{u : \Re\{u\} = ct\}$, A_k are the weights and u_k the nodes (both complex quantities). Formula (7.3.15) is the N -point Gauss quadrature formula and is called the G_N -rule. This formula has a number of shortcomings, namely, (i) there

is no procedure to determine N a priori for a desired accuracy, which leads to using this formula successively with increasing order and finding an agreement between two consecutive approximations to desired accuracy; (ii) this procedure then uses different values of nodes of different order in each approximation; and (iii) when N is large, the weights also become large, which leads to considerable cancellation errors. To avoid these shortcomings, Piessens (1969c) has developed the following approximation:

$$tf(t) = \frac{1}{2i\pi} \int_{L'} e^u u^{-\gamma} G(u) du \approx \sum_{k=1}^N B_k G(u_k) + \sum_{k=1}^{N+1} C_k G(v_k), \quad (7.3.16)$$

where u_k are the nodes of the G_N -rule (7.3.15), such that the precision in (7.3.16) is maximum. Formula (7.3.16) is a $2N + 1$ -point Gauss quadrature formula and is called the G_N^* -rule. The nodes u_k , $k = 1, 2, \dots, N$, are the zeros of the polynomial in $P_N(1/s)$ defined by

$$P_N(1/s) = (-1)^N e^{-s} s^{N+\gamma-1} \frac{d^N}{ds^N} \left(\frac{e^s}{s^{N+\gamma-1}} \right),$$

or

$$P_N(1/s) = (-1)^N {}_2F_0(-N, N + \gamma - 1; 1/s). \quad (7.3.17)$$

These polynomials are such that $\frac{1}{2i\pi} \int_{L'} e^s s^{-\gamma} P_N(1/s) s^{-r} ds = 0$ for $r = 0, 1, \dots, N - 1$.

Now, the orthogonality property of the polynomials implies that there also exists a polynomial $Q_K(1/s)$ of degree K such that

$$\frac{1}{2i\pi} \int_{L'} e^s s^{-\gamma} P_N(1/s) Q_K(1/s) s^{-r} ds = 0 \quad \text{for } r = 0, 1, \dots, K - 1. \quad (7.3.18)$$

The weights B_k and C_k in formula (7.3.16) can be determined so that the degree of precision in this formula is $N + 2K - 1$, provided that the nodes v_k are the zeros of the polynomial $Q_K(1/s)$. To determine the polynomials $Q_K(1/s)$, we first calculate the moments for the case $\gamma = 1$. Thus, the r -th moment is

$$M_{N,r} = \frac{1}{2i\pi} \int_{L'} e^s s^{-1} P_N(1/s) s^{-r} ds, \quad (7.3.19)$$

where $M_{N,r} = 0$ for $r = 0, 1, \dots, N - 1$, and

$$M_{N,N+k} = \frac{(-1)^N (N+k)!}{k! (2N+k)!} \quad \text{for } k = 0, 1, 2, \dots \quad (7.3.20)$$

If we set

$$Q_K(1/s) = \frac{1}{s^K} + \frac{a_{K-1}}{s^{K-1}} + \dots + \frac{a_1}{s} + a_0, \quad (7.3.21)$$

and substitute this into (7.3.18), we find that there exists a solution only if K is at least $N + 1$. Hence, we will take $K = N + 1$. The coefficients a_k , $k = 0, 1, \dots, N$, in (7.3.21) are computed recursively by

$$\begin{aligned} a_N &= -\frac{M_{N,N+1}}{M_{N,N}}, \\ a_{N-k} &= -\frac{M_{N,N+k+1} + M_{N,N+k} a_N + \dots + M_{N,N+1} a_{N-K+1}}{M_{N,N}}, \\ &\text{for } k = 1, 2, \dots, N, \end{aligned}$$

which, in view of the definition (7.3.19) yield the recursive formula

$$\begin{aligned} a_N &= -\frac{N+1}{2N+1}, \\ a_{N-k} &= -[C_{N,k+1} + C_{N,k} a_N + \dots + C_{N,1} a_{N-k+1}], \quad k = 1, 2, \dots, N, \end{aligned} \quad (7.3.22)$$

where

$$C_{N,i} = \frac{M_{N,N+i}}{M_{N,N}} = \frac{(N+1)(N+2)\dots(N+i)}{(2N+1)(2N+2)\dots(2N+i)i!}.$$

The additional nodes v_k in the new G_N^* -rule (7.3.16) are the zeros of $Q_{N+1}(1/s)$, and the weights B_k and C_k are given by

$$\begin{aligned} B_k &= \frac{(-1)^N (2N-1)(N-1)!}{u_k^2 P_{N-1}(1/u_k) Q_{N+1}(1/u_k) (2N)!} + A_k, \\ A_k &= \frac{(-1)^{N+1} (2N-1)^2}{N u_k^2 [P_{N-1}(1/u_k)]^2}, \\ C_k &= \frac{(-1)^N N!}{P_N(1/v_k) Q'_{N+1}(1/v_k) (2N)!}, \end{aligned}$$

where the prime denotes the derivative with respect to $1/s$. The weights B_k are almost as large as A_k , but C_k are much smaller than A_k . Thus, the round-off error in both G_N -rule and the new G_N^* -rule is almost the same. The nodes and weights of the G_N^* -rule for $N = 2(1)12$ are available in [Table A.31](#) (Piessens 1969c).

Several authors have tabulated tables of the weights A_k and the nodes u_k . For example, Salzer (1955) gives u_k , their inverses, and the products $u_k A_k$ to between 4S* and 8S for $N = 1(1)8$ and $\gamma = 1$; Salzer (1961) gives the same quantities to between 12S and 15S for $N = 1(1)16$ and $\gamma = 1$; Krylov and Skoblya (1961) give A_k and u_k to 5S to 7S for $N = 1(1)9$ and for values of γ which are integer multiples of $\frac{1}{4}$ and $\frac{1}{3}$ between the limits $\frac{1}{4}$ and 3; in 1969 they also give A_k and

*Here S stands for 'significant digits'.

u_k to 20S for $N = 1(1)15$ and $\gamma = 1(1)5$, and to 7S to 8S for $N = 1(1)10$ and $\gamma = 0.01(0.01)3.0$; Skoblya (1964) gives u_k to 8S and A_k to 7S for $N = 1(1)10$ and $\gamma = 0.1(0.1)3.0$; Stroud and Secrest (1966) give u_k and A_k to 30S for $N = 2(1)24$ and $\gamma = 1$; and Piessens (1969b) gives u_k and A_k to 16S for $N = 6(1)12$ and $\gamma = 0.1(0.1)3.0, 3.5, 4.0, \frac{1}{3}, \frac{2}{3}, \frac{4}{3}, \frac{5}{3}, \frac{7}{3}, \frac{8}{3}, \frac{10}{3}, \frac{1}{4}, \frac{3}{4}, \frac{5}{4}, \frac{7}{4}, \frac{9}{4}, \frac{1}{6}, \frac{1}{7}, \frac{1}{8}, \frac{1}{9}$.

EXAMPLE 7.3.3. Piessens (1969c) considers $\bar{f}(s) = \frac{1}{\sqrt{s^2+1}}$, for which $f(t) = J_0(t)$. The result obtained from both G_N and G_N^* rules are given in Table 7.3.3. It is obvious that the accuracy increases for the G_N^* -rule with larger N . ■

EXAMPLE 7.3.4. Piessens (1971) considers $\bar{f}(s) = \frac{e^{1/\sqrt{s}}}{\sqrt{s}}$, which has the indicial function

$$f(t) = \frac{1}{2t\sqrt{\pi t}} \int_0^\infty u e^{-u^2/4t} J_0(2\sqrt{u}) du.$$

Using the approximation

$$f(t) \approx \frac{1}{\sqrt{t}} \sum_{k=1}^6 \left[A_k^{(0.5)} G_1(u_k^{(0.5)}) - A_k^{(1.0)} G_2(u_k^{(1.0)}) \right],$$

where $G_1(x) = \cosh \sqrt{t/x}$ and $G_2(x) = \sqrt{x/t} \sinh \sqrt{t/x}$, and using the values of $A_k^{(\alpha)}$ and $u_k^{(\alpha)}$ from the tables given in Piessens (1969b) for $\gamma = \alpha$ and $N = 6$, this example is solved numerically and the results are available in Piessens (1971). ■

TABLE 7.3.3.

t	G_5	G_5^*	G_8	G_8^*	Exact
1	0.76518	0.76519	0.76525	0.76519	0.7651976865579666
2	0.22389	0.22390	0.22403	0.22405	0.2238907791412356
4	-0.39701	-0.39718	-0.39732	-0.39722	-0.3971498098638473
6	0.13883	0.15068	0.15104	0.15077	0.1506452572509970
8	0.21100	0.16728	0.17162	0.17160	0.1716508071375542
10	-0.07542	-0.19675	-0.24436	-0.24579	-0.2459357644513483
12			0.02722	0.04762	0.0476893107968335

7.3.4. Kajiware and Tsuji's Method. The polynomials $p_N(\xi)$, defined by (7.1.5), are used to approximate $\bar{f}(s)$ by using the Clenshaw-Curtis quadrature rule (§3.3.1). Since the polynomials $p_N(\xi)$ oscillate with larger amplitudes as the value of N increases, Kajiware and Tsuji (1995a) use the technique of changing them

to the logarithm by setting

$$\begin{aligned} A(n, k) &= \ln \frac{(2n)!}{(n+1)! k! (n+k)!} \\ &= \left(\sum_{i=1}^{2n} - \sum_{i=1}^{2+1} - \sum_{i=1}^k - \sum_{i=1}^{n-k} - \sum_{i=1}^{n+k} \right) \ln j. \end{aligned} \quad (7.3.23)$$

Then the polynomials $p_N(\xi)$ are computed from

$$\begin{aligned} p_N(\xi) &= \sum_{0 \leq k \leq n \leq N} (-1)^{k+1} \left[\exp \left\{ \frac{A(n, k)}{n+k} \right\} \exp \left\{ \frac{\xi}{n+k} \right\} \xi \right]^{n+k} \\ &\quad \times \left\{ \frac{2n+1}{n+k+1} \xi^2 - \left(\frac{2n+1}{n+k+1} + 3n+1 \right), \xi + n(n+k+1) \right\}. \end{aligned} \quad (7.3.24)$$

The inverse $\bar{f}(s)$ is then approximated by the inverse Laplace transform of $f_N(t)$, which is written as

$$f_N(t) = \int_0^\infty f(s) e^{-st} p_N(st) ds = \frac{1}{t} \int_0^\infty f(s/t) e^{-s} p_N(s) ds. \quad (7.3.25)$$

The round-off error caused by addition is estimated by taking $\delta_0 = 0$,

$$\delta_j = \epsilon_M \max \{ |a_j|, |p_j|, |p_{j-1}| \} + \delta_{j+1},$$

where ϵ_M is the machine precision; the index j stands for the j -th pair in order of $(n, k) = (N, N), (N, N-1), \dots, (N, 0), (N-1, N-1), (N-1, N-2), \dots, (1, 1), (1, 0), (0, 0)$; the quantities a_k are the computed values of

$$(-1)^{k+1} A(n, k) \left\{ \frac{2n+1}{n+k+1} s^2 - \left(\frac{2n+1}{n+k+1} + 3n+1 \right) s + n(n+k+1) \right\};$$

and $p_0 = 0$, $p_j = p_{j-1} + a_j$ for $j = 1(1)M$, where $M = (N+1)(N+2)/2$. The values of p_M are computed for $s = 50$ and $N = 40$, which are presented in [Table A.32](#). Neglecting the truncation error $\varepsilon(t)$, the round-off error is computed by $\delta(s, t) = \delta_M(s) \frac{1}{t} f(1/t)$; the error due to the oscillation of the polynomials p_N is controlled by $D = \sqrt{\int_0^\infty \delta(t)^2 dt}$, where $\delta(t) = \int_0^\infty \delta(s, t) ds + \varepsilon(t)$. The transformation of $f_N(t)$, given by (7.3.25), enables fast storage of the computed values of $p_N(s)$. The Clenshaw-Curtis rule is used to compute the approximate values of $f_N(t)$. Kajiwara and Tsuji (1995b) have provided a Fortran77 program to compute $p_N(s)$ using an algorithm that eliminates round-off errors of addition and multiplication. Some results

are given in Table 7.3.4, where $G_N = \sqrt{\int_0^\infty |f(t) - f_N(t)|^2 dt}$, and the total error is the sum of D and the truncation error.

Table 7.3.4.

N	$f_N(1)$	G_N	D	Total Error
10	0.13863534	2.91735(-02)	6.551(-12)	4.083(-05)
20	0.14899286	1.74395(-02)	2.016(-09)	5.939(-05)
30	0.15301003	1.24817(-02)	1.118(-06)	7.226(-05)
35	0.15420178	1.09448(-02)	2.143(-03)	2.146(-03)
36	0.15490459	3.80202(-02)	7.384(-03)	7.563(-03)
38	0.14087664	—	—	—
40	0.84248827	—	—	—

7.4. Use of Fourier Series

A Fourier series representation of an unknown function $f(t)$ can be used effectively for numerical evaluation of the function $f(t)$. We discuss the methods of Dubner and Abate (1968) and Durbin (1974).

7.4.1. Dubner and Abate's Method. Setting $s = c + i\omega$ in (7.1.1), we get

$$\int_0^\infty e^{-(c+i\omega)t} f(t) dt = \bar{f}(s),$$

whose real and imaginary parts

$$\Re\{\bar{f}(s)\} = \int_0^\infty e^{-ct} f(t) \cos \omega t dt, \quad \Im\{\bar{f}(s)\} = -\int_0^\infty e^{-ct} f(t) \sin \omega t dt,$$

are known as the Fourier cosine and sine transform of $f(t)$, respectively. Note that $a > a_0$, where a_0 is a real constant such that all singularities of $\bar{f}(s)$ lie to the left of $\Re\{s\} = a_0$. Using the Fourier inversion formula we obtain

$$f(t) = \frac{2e^{ct}}{\pi} \int_0^\infty \Re\{\bar{f}(s)\} \cos \omega t d\omega = -\frac{2e^{ct}}{\pi} \int_0^\infty \Im\{\bar{f}(s)\} \sin \omega t d\omega. \quad (7.4.1)$$

Thus, the problem reduces to numerically evaluate either of the integrals in (7.4.1).

Consider a real function $h(t)$ such that $h(t) = 0$ for $t < 0$. Divide the interval $[0, \infty)$ into subintervals of length T , where the n -th subinterval is $(nT, (n+1)T)$. The entire range $[0, \infty)$ is covered as $n \rightarrow \infty$. Consider the function $h(t)$ in the

interval $((n-1)T, (n+1)T)$, and define even periodic functions $g_n(t)$ of period $2T$ such that

$$g_n(t) = \begin{cases} h(t) & \text{if } nT \leq t \leq (n+1)T, \\ h(2nT - t) & \text{if } (n-1)T \leq t \leq nT. \end{cases} \quad (7.4.2)$$

After replacing t by $nT + t$ on the right side of (7.4.2), we have for even values of n

$$g_n(t) = \begin{cases} h(nT + t) & \text{if } 0 \leq t \leq T, \\ h(nT - t), & \text{if } -T \leq t \leq 0; \end{cases}$$

and for odd values of n

$$g_n(t) = \begin{cases} h((n+1)T - t) & \text{if } 0 \leq t \leq T, \\ h((n+1)T + t) & \text{if } -T \leq t \leq 0. \end{cases}$$

Thus, the Fourier series for each $g_n(t)$ is

$$g_n(t) = \frac{A_{n,0}}{2} + \sum_{k=1}^{\infty} A_{n,k} \cos(\omega_k t), \quad \omega_k = k\pi/T,$$

where

$$A_{n,k} = \begin{cases} \frac{2}{T} \int_0^T h(nT + x) \cos(\omega_k t) dx & \text{for } n = 0, 2, 4, \dots, \\ \frac{2}{T} \int_0^T h((n+1)T - x) \cos(\omega_k t) dx & \text{for } n = 1, 3, 5, \dots, \end{cases}$$

or

$$A_{n,k} = \frac{2}{T} \int_{nT}^{(n+1)T} h(x) \cos(\omega_k t) dx.$$

Thus,

$$\sum_{n=0}^{\infty} g_n(t) = \frac{2}{T} \left[\frac{A(\omega_0)}{2} + \sum_{k=1}^{\infty} A(\omega_k) \cos \omega_k t \right], \quad (7.4.3)$$

where $A(\omega_k) = \int_0^{\infty} h(t) \cos \omega_k t dt$. If $h(t) = e^{-ct} f(t)$, then Eq (7.4.3) represents the Laplace transform of the real-valued function $f(t)$ with the transform parameter $s = c + i\omega_k$. This implies that $A(\omega_k) = \Re\{\bar{f}(s)\}$. Then, multiplying both sides of Eq (7.4.3) by e^{ct} , we get

$$\sum_{n=0}^{\infty} e^{ct} g_n(t) = \frac{2e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t \right]. \quad (7.4.4)$$

Since the first term in the sum on the left side is $e^{ct} g_0(t) = f(t)$ in the interval $0 \leq t \leq T$, the rest of the terms $\sum_{n=1}^{\infty} e^{ct} g_n(t)$ represent the error which in the interval

$(0, T)$ is given by

$$\begin{aligned} E &= \sum_{n=1}^{\infty} e^{ct} g_n(t) = e^{ct} \sum_{n=1}^{\infty} [h(2n+t) + h(2n-t)] \\ &= \sum_{n=1}^{\infty} e^{-2cnT} [f(2n+t) + e^{2ct} f(2n-t)]. \end{aligned} \quad (7.4.5)$$

If we apply the trapezoidal rule to Eq (7.4.1) with step size π/T , we obtain the approximation

$$f(t) \approx \frac{2e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_1^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t \right]. \quad (7.4.6)$$

Note that the above error estimate depends not only on the step size but also on c which can be chosen appropriately in order to minimize the error. The error can be made reasonably small only for $t \leq T/2$. Thus, formulas (7.4.3) and (7.4.6) compute $\mathcal{L}^{-1}\{\bar{f}(s)\}$ to a desired accuracy in the interval $(0, T/2)$. In fact, since c is chosen such that no singularities of $\bar{f}(s)$ lie to the right of $\Re\{s\} = c$, we will assume that no singularities of $\bar{f}(s)$ lie to the right of the origin, which is always possible by a translation of the origin and an adjustment to $\bar{f}(s)$. Let us assume that $f(t)$ is bounded by some function of the type Ct^m , where C is a constant and m is a nonnegative integer. First, we consider $m = 0$; then from Eq (7.4.5) we have

$$\text{error} = E_1 \leq C e^{c(t-T)} \frac{\cosh ct}{\sinh cT}.$$

Clearly, the error becomes large as $t \rightarrow T$. Therefore, we should limit the use of formula (7.4.6) to the interval $(0, T/2)$. Then the error in this interval is restricted to $C e^{-cT/2}$. Also, if $f(t) \leq Ct^m$ for $m > 0$, then the error in the interval $(0, T/2)$ is bounded by

$$E_1 \leq C e^{-cT/2} \frac{\cosh cT/2}{\sinh cT} \approx C (1.5T)^m e^{-cT}.$$

Thus, this method reduces to the following steps: First, determine the interval for which the evaluation is needed, say, $0 \leq t \leq t_1$; then take $T = 2t_1$, and determine a from (7.4.5) so that the error is within tolerance.

EXAMPLE 7.4.1. Consider $\bar{f}(s) = \frac{1}{s^2 + s + 1}$ for which the exact solution is $f(t) = \frac{2}{\sqrt{3}} e^{-t/2} \sin \sqrt{3}t/2$. [Table 7.4.1](#) presents exact values $f(t)$ (column 2) and approximate values from formula (7.4.6) using $\bar{f}(s)$ (column 3, for $cT = 8$, $T = 20$,

by taking the first 2000 terms in formula (7.4.6). ■

Table 7.4.1

t	$f(t)$	Exact	t	$f(t)$	Exact
0.0	0.0000	0.0020	1.5	0.5254	0.5254
0.5	0.3773	0.3773	2.0	0.4193	0.4193
1.0	0.5335	0.5335	10.0	0.0054	0.0054

EXAMPLE 7.4.2. Consider $\bar{f}(s) = \frac{1}{s^2 + 1}$ for which $f(t) = \sin t$. Table 7.4.2 gives exact values for $f(t)$ (column 2) and approximate values from formula (7.4.6) using $\bar{f}(s)$ (column 3). If we use the same values of a and T as in Example 7.4.1 with the first 2000 terms, then the error, according to formula (7.4.5), appears in the fourth decimal digit near $T/2$. Note that the function $f(t)$ converges very slowly. ■

Table 7.4.2

t	$f(t)$	Exact	t	$f(t)$	Exact
0.00	0.0000	0.0020	1.50	0.9974	0.9974
0.25	0.2474	0.2474	1.75	0.9839	0.9839
0.50	0.4794	0.4794	2.00	0.9092	0.9092
0.75	0.6816	0.6816	4.00	−0.7568	−0.7568
1.00	0.8414	0.8414	9.00	0.4121	0.4120
1.25	0.9489	0.9489	10.00	−0.5440	−0.5443

7.4.2. Crump’s Improvement. This method is an improvement upon the above Dubner and Abate’s method; it uses both Fourier cosine and sine series, requires, besides the transform function itself, only the cosine, sine and exponential functions. It differs from the Dubner and Abate’s method in two respects: (i) The Fourier series contains additional terms involving the sine function selected in such a manner that the approximating function is less than the approximating function (7.4.6) and that the Fourier series approximates the original function $f(t)$ on an interval of twice the length of the interval taken in (7.4.6); and (ii) Crump’s method uses a transformation of the approximating series into one that converges very rapidly.

Crump (1976) has proved the following result: Let $f(t)$ be a real-valued function which is piecewise continuous for $t \geq 0$, and of exponential order α . Then the

function $f(t)$ is defined by (7.4.1), and for $c > \alpha$, $0 \leq t < 2T$, we have

$$f(t) = \frac{e^{ct}}{T} \left[\frac{1}{2} \bar{f}(c) + \sum_{j=1}^{\infty} \left\{ \Re \bar{f}\left(c + \frac{j\pi i}{T}\right) \cos \frac{j\pi t}{T} \right. \right. \\ \left. \left. - \Im \bar{f}\left(c + \frac{j\pi i}{T}\right) \sin \frac{j\pi t}{T} \right\} \right] - e^{ct} \sum_{n=1}^{\infty} \{e^{-c(2nT+t)} f(2nT+t)\}. \quad (7.4.7)$$

For proof, define a function $k_n(t)$, $n = 0, 1, 2, \dots$, such that $k_n(t) = e^{-ct} f(t)$ for $2nT \leq t < 2(n+1)T$, and elsewhere $k_n(t)$ is a periodic function of period $2T$. Then the Fourier series of $k_n(t)$ is

$$k_n(t) = \frac{1}{2} A_{n,0} + \sum_{j=1}^{\infty} \left[A_{n,j} \cos \frac{j\pi t}{T} + B_{n,j} \sin \frac{j\pi t}{T} \right],$$

where

$$A_{n,j} = \frac{1}{T} \int_{2nT}^{2(n+1)T} e^{-ct} f(t) \cos \frac{j\pi t}{T} dt, \quad (7.4.8)$$

$$B_{n,j} = \frac{1}{T} \int_{2nT}^{2(n+1)T} e^{-ct} f(t) \sin \frac{j\pi t}{T} dt. \quad (7.4.9)$$

Thus,

$$\sum_{n=0}^{\infty} k_n(t) = \sum_{n=0}^{\infty} \left[\frac{1}{2} A_{n,0} + \sum_{j=1}^{\infty} \left\{ A_{n,j} \cos \frac{j\pi t}{T} + B_{n,j} \sin \frac{j\pi t}{T} \right\} \right]. \quad (7.4.10)$$

Substituting (7.4.8) and (7.4.9) into the series (7.4.10), we find after inverting the order of summation that

$$\begin{aligned} \sum_{n=0}^{\infty} k_n(t) &= \frac{1}{2T} \int_0^{\infty} e^{-ct} f(t) dt \\ &\quad + \frac{1}{T} \sum_{j=1}^{\infty} \sum_{n=0}^{\infty} \left[\left\{ \int_{2nT}^{2(n+1)T} e^{-ct} f(t) \cos \frac{j\pi t}{T} dt \right\} \cos \frac{j\pi t}{T} \right. \\ &\quad \left. + \left\{ \int_{2nT}^{2(n+1)T} e^{-ct} f(t) \sin \frac{j\pi t}{T} dt \right\} \sin \frac{j\pi t}{T} \right] \\ &= \frac{1}{2T} \int_0^{\infty} e^{-ct} f(t) dt \\ &\quad + \frac{1}{T} \sum_{j=1}^{\infty} \left\{ \int_0^{\infty} e^{-ct} f(t) \cos \frac{j\pi t}{T} dt \cos \frac{j\pi t}{T} \right. \\ &\quad \left. + \int_0^{\infty} e^{-ct} f(t) \sin \frac{j\pi t}{T} dt \sin \frac{j\pi t}{T} \right\}. \quad (7.4.11) \end{aligned}$$

Substituting for the integrals in (7.4.11) from the definition of Fourier cosine and sine transforms of $f(t)$, we get

$$\sum_{n=0}^{\infty} k_n(t) = \frac{1}{T} \left\{ \frac{1}{2} \bar{f}(c) + \sum_{j=1}^{\infty} \left\{ \Re \bar{f}\left(c + \frac{j\pi i}{T}\right) \cos \frac{j\pi t}{T} - \Im \bar{f}\left(c + \frac{j\pi i}{T}\right) \sin \frac{j\pi t}{T} \right\} \right\}. \quad (7.4.12)$$

Since

$$\sum_{n=0}^{\infty} k_n(t) = e^{-ct} f(t) + \sum_{n=1}^{\infty} e^{-c(2nT+t)} f(2nT+t) \quad \text{on } [0, 2T],$$

we find, on comparing this to (7.4.12) that

$$e^{-ct} f(t) + \sum_{n=1}^{\infty} e^{-c(2nT+t)} f(2nT+t) = \frac{1}{T} \left[\frac{1}{2} \bar{f}(c) + \sum_{j=1}^{\infty} \left\{ \Re \bar{f}\left(c + \frac{j\pi i}{T}\right) \cos \frac{j\pi t}{T} - \Im \bar{f}\left(c + \frac{j\pi i}{T}\right) \sin \frac{j\pi t}{T} \right\} \right],$$

which, after solving for $f(t)$ for $0 \leq t < 2T$, yields $f(t) = f^*(t) - E$, where the $f^*(t)$ is the approximate solution

$$f^*(t) = \frac{e^{ct}}{T} \left[\frac{1}{2} \bar{f}(c) + \sum_{j=1}^{\infty} \left\{ \Re \bar{f}\left(c + \frac{j\pi i}{T}\right) \cos \frac{j\pi t}{T} - \Im \bar{f}\left(c + \frac{j\pi i}{T}\right) \sin \frac{j\pi t}{T} \right\} \right], \quad (7.4.13)$$

and E the error, given by

$$E = e^{ct} \sum_{n=1}^{\infty} e^{-c(2nT+t)} f(2nT+t). \quad (7.4.14)$$

The approximating formula (7.4.13) for the integral (7.1.1) is essentially a trapezoidal rule approximation.

Ignoring the round-off error, there are two sources of errors in Crump's formula (7.4.13): (i) the Fourier coefficients used in the Fourier series for $k_0(t)$ are only approximations obtained by using $\bar{f}(s)$; and (ii) there is truncation error since the series in (7.4.13) are not summed to infinity. The error bound is given by

$$E \leq M e^{ct} \frac{1}{E^{2T(c-\alpha)} - 1}, \quad 0 < t < 2T. \quad (7.4.15)$$

If we choose a sufficiently larger α in (7.4.14), the error E can be made as small as desired. If, e.g., in applying formula (7.4.13) we want convergence to at least 4

significant digits, we must require that the relative error $E_R \equiv (E/M) e^{\alpha t} \leq 0.00005$, which means that we can replace (7.4.14) by $E \leq M e^{\alpha t} e^{-2T(c-\alpha)}$ for $0 \leq t < 2T$.

There are three cases of instability: (i) If the error is at $t = 0$, it is usually due to a discontinuity in the Fourier series expansion for $k_0(t)$ at $t = 0$, which is $k_0(0) = \frac{1}{2} \{f(0) + f(2T) e^{2cT}\}$. Hence from (7.4.13) and (7.4.14) we find that $f^*(0) - \frac{1}{2} f(0) = E + \frac{1}{2} f(2T) e^{-2cT} \leq M e^{-2T(c-\alpha)} + \frac{1}{2} M e^{-2T(c-\alpha)} = \frac{3}{2} E$. Thus, at $t = 0$ formula (7.4.13) approximates $\frac{1}{2} f(0)$ rather than $f(0)$ with an error bound 50% greater than that for $t > 0$. (ii) If the error is at a value of t close to zero, the error bound (7.4.15) provides an algorithm for computing $f(t)$ to a predetermined accuracy; and (iii) if the error is at extremely small values of t , which deviate from the exact value, the instability is due to the situation where the approximation $f^*(t)$ approaches $\frac{1}{2} [f(2T) + f(0)]$ instead of the Fourier series converging to $k_0(t)$ at the points of discontinuity under the condition $f(t) = \frac{1}{2} [f(t+) + f(t-)]$. Some of the following examples clearly exhibit such an instability.

EXAMPLE 7.4.3. Crump (1976) considers the following four transforms:

$$(i) \bar{f}_1(s) = \frac{s-1}{(s-1)^2+1} - \frac{1}{s}, \text{ for which } f(t) = e^t \cos t - 1;$$

$$(ii) \bar{f}_2(s) = \frac{2}{s} - \frac{1}{s+1}, \text{ for which } f(t) = 2 - e^{-t};$$

$$(iii) \bar{f}_3(s) = \left(\frac{2}{s} - \frac{1}{s+1}\right) e^{-5s}, \text{ for which } f(t) = \begin{cases} 0, & t > 5, \\ 2 - e^{5-t}, & t \leq 5; \end{cases}$$

$$(iv) \bar{f}_4(s) = \frac{1}{s^2+s+1}, \text{ for which } f(t) = \frac{2}{\sqrt{3}} e^{-t/2} \sin \frac{t\sqrt{3}}{2}.$$

Both Euler transformation (ET) and ϵ -algorithm (EPAL) are used for rapid convergence (for ET and EPAL see [algorithms.pdf](#) on the CD-R). As a result of computation of these inversions by formula (7.4.13) Crump has found that

In (i) the Euler transformed series converges faster than the untransformed series, but EPAL gives more uniform accuracy.

In (ii) smaller values of T improve convergence for small t but show the opposite effect for large t . Convergence is usually the best for t near T . One must take $2T > t_{\max}$ in order to control the relative error, and if $2T$ is too close to t_{\max} convergence is very slow for larger values of t . The best choice of T appears to be 7.5 for relative error of 10^{-8} , and 6 for relative error of 10^{-4} . Generally, the smaller T is, the smaller the relative error is.

In (iii) EPAL makes convergence faster and gives the best results. The computed values confirm the predicted perturbation in the neighborhood of the discontinuity at $t = 5$, which is due to the Gibbs phenomenon. This discontinuity can be removed by inverting $\bar{f}_3^*(s) = \bar{f}_3(s) - e^{-5s}/s$, and then taking $f_3(t) = \begin{cases} f_3^*(t), & T < 5, \\ f_3^*(t) + 1, & t \geq 5. \end{cases}$ This procedure not only removes the singularity but generally hastens convergence,

and the error remains relatively lower in the neighborhood of $t = 5$, due to the nonexistence of the first derivative.

In (iv) the results obtained with ET are compared to those of Dubner and Abate discussed in §7.4.1.

EXAMPLE 7.4.4. Haines (1982) uses Crump’s formula (7.4.13) and considers the three test cases:

- (i) $\bar{f}_1(s) = e^{-a\sqrt{s}}$, with $a = 0.1$, for which $f_1(t) = \frac{ae^{-a^2/(4t)}}{2\sqrt{\pi t^3}}$;
- (ii) $\bar{f}_2(s) = \frac{e^{-a\sqrt{s}}}{\sqrt{s}}$, with $a = 1.0, 0.1, 0.05$, for which $f_2(t) = \frac{e^{-a^2/(4t)}}{\sqrt{\pi t}}$; and
- (iii) $\bar{f}_3(s) = \frac{\sqrt{s+b}e^{-a\sqrt{s+b}}}{s}$, with $a = 1.0, 0.5, 0.1$ and $b = 0.5, 0.1$, for which $f_3(t) = \frac{e^{-a^2/(4t)+bt}}{\sqrt{\pi t}} - \frac{\sqrt{b}}{2} \left[e^{a\sqrt{b}} \operatorname{erfc}\left(\frac{a}{2\sqrt{t}} + \sqrt{bt}\right) + e^{-a\sqrt{b}} \operatorname{erfc}\left(\frac{a}{2\sqrt{t}} - \sqrt{bt}\right) \right]$.

The ϵ -algorithm is used to accelerate convergence. For ϵ -algorithm and related codes, see the file [algorithms.pdf](#) on the CD-R.

The results for some selected values of a and b are shown in Tables 7.4.4(i)–7.4.4(iii); other tables can be found in Haines (1982). The results in these tables are obtained for very small values of t ; they exhibit instability for very small values of t ; for example, in Table 7.4.4(i) the instability for accuracy in the fifth decimal digit starts at $t = 0.2(-3)$.

Table 7.4.4(i). Example 7.4.4(i) with $a = 1$.

t	$f_1^*(t)$	$f_1(t)$
0.3(−3)	0.13049460(+1)	0.13049464(+1)
0.2(−3)	0.37167999(−1)	0.37168004(−1)
0.1(−3)	0.40281254(−6)	0.39177183(−6)
0.9(−4)	0.39198591(−7)	0.28529613(−7)
0.8(−4)	0.12263991(−7)	0.10569580(−7)
0.7(−4)	−0.27260081(−8)	−0.14867262(−10)
0.6(−4)	0.10158857(−7)	0.48704037(−13)
0.5(−4)	0.30174193(−7)	0.15389204(−14)
0.4(−4)	0.17049456(−8)	0.80149376(−22)
0.3(−4)	0.13077603(−10)	0.11053671(−30)
0.2(−4)	0.78363141(−15)	0.16294452(−48)
0.1(−4)	0.69315321(−23)	0.23810843(−102)

Table 7.4.4(ii). Example 7.4.4(ii) with $a = 0.1$.

t	$f_1^*(t)$	$f_1(t)$
0.5(+1)	0.25218725(+0)	0.25206117(+0)
0.3(+1)	0.32546384(+0)	0.32519271(+0)
0.1(+1)	0.56273116(+0)	0.56137591(+0)
0.9(+0)	0.59305866(+0)	0.59141352(+0)
0.7(+0)	0.67193183(+0)	0.66953629(+0)
0.5(+0)	0.79390550(+0)	0.78994532(+0)
0.3(+0)	0.10215169(+1)	0.10150395(+1)
0.1(+0)	0.17400748(+1)	0.16971121(+1)
0.9(-1)	0.18291120(+1)	0.17790023(+1)
0.7(-1)	0.20576227(+1)	0.19854328(+1)
0.5(-1)	0.24000792(+1)	0.22830257(+1)
0.3(-1)	0.29969084(+1)	0.27572085(+1)
0.1(-1)	0.43939158(+1)	0.34219842(+1)
0.9(-2)	0.45047091(+1)	0.34121592(+1)
0.7(-2)	0.47181489(+1)	0.33011547(+1)
0.5(-2)	0.48394184(+1)	0.29352545(+1)
0.3(-2)	0.44766462(+1)	0.19455414(+1)
0.1(-2)	0.14644984(+1)	0.12021339(+0)
0.9(-3)	0.11693117(+1)	0.72708760(-1)
0.7(-3)	0.59954654(+0)	0.16856709(-1)
0.5(-3)	0.17996755(+0)	0.11455069(-2)
0.3(-3)	0.78296866(-2)	0.19828159(-5)
0.1(-3)	0.31563134(-7)	0.10831810(-19)
0.9(-4)	0.19072069(-7)	0.44343767(-22)

Table 7.4.4(iii). Example 7.4.4(iii) with $a = 0.5$ and $b = 0.1$.

t	$f_2^*(t)$	$f_2(t)$
0.6(-2)	0.21789604(-3)	0.21787624(-3)
0.5(-2)	0.29731833(-4)	0.29720595(-4)
0.4(-2)	0.15438832(-5)	0.14688921(-5)
0.3(-2)	0.34331774(-7)	0.92244034(-8)
0.2(-2)	0.19941938(-8)	0.33816683(-12)
0.1(-2)	0.10700834(-11)	0.12822632(-25)

continued next page

Table 7.4.4(iii). Example 7.4.4(iii) with $a = 0.5$ and $b = 0.1$, Continued.

t	$f_2^*(t)$	$f_2(t)$
0.9(−3)	0.19269665(−12)	0.13027455(−28)
0.8(−3)	0.22469598(−13)	0.23474122(−32)
0.7(−3)	0.14041946(−14)	0.35690526(−37)
0.6(−3)	0.35624924(−16)	0.21787624(−3)
0.9(−3)	0.21789604(−3)	0.13283579(−43)

7.4.3. Durbin’s Improvement. Durbin (1974) improved upon the above method by constructing an infinite set of functions $k_n(t)$ with period $2T$ for $n = 0, 1, 2, \dots$, as follows:

$$k_n(t) = \begin{cases} h(t) & \text{if } nT \leq t \leq (n + 1)T, \\ -h(2nT - t) & \text{if } (n - 1)T \leq t \leq nT. \end{cases} \tag{7.4.16}$$

For example, $k_n(t)$ in the intervals $(-T, 0)$, $(0, T)$, and $(T, 2T)$ for even and odd values of n , respectively, is given by

$$k_n(t) = \begin{cases} -h(nT - t) & \text{if } -T \leq t \leq 0, \\ h(nT + t) & \text{if } 0 \leq t \leq T, \\ -h(nT - t) & \text{if } T \leq t \leq 2T, \end{cases} \quad \text{for } n = 0, 2, 4, \dots; \tag{7.4.17}$$

$$k_n(t) = \begin{cases} h((n + 1)T + t) & \text{if } -T \leq t \leq 0, \\ -h((n + 1)T - t) & \text{if } 0 \leq t \leq T, \\ h((n - 1)T + t) & \text{if } T \leq t \leq 2T, \end{cases} \quad \text{for } n = 1, 3, 5, \dots. \tag{7.4.18}$$

The Fourier series representation for each $k_n(t)$ is

$$k_n(t) = \sum_{k=0}^\infty B_{n,k} \sin \omega_k t, \tag{7.4.19}$$

where

$$B_{n,k} = \int_{nT}^{(n+1)T} e^{-ct} f(t) \sin \omega_k t \, dt. \tag{7.4.20}$$

Summing $B_{n,k}$ in (7.4.20) over n and using the Fourier integrals for $\Re\{\bar{f}(s)\}$ and $\Im\{f(s)\}$, we get

$$\sum_{n=0}^\infty B_{n,k} = \frac{2}{T} \int_0^\infty e^{-ct} f(t) \sin \omega_k t \, dt = -\frac{2}{T} \Im\{\bar{f}(c + i\omega_k)\}, \tag{7.4.21}$$

which, after multiplying both sides of (7.4.21) by $e^{ct} \sin \omega_k t$ and using (7.4.19), gives

$$\sum_{n=0}^{\infty} e^{ct} k_n(t) = \sum_{n=0}^{\infty} B_{n,k} e^{ct} \sin \omega_k t = -\frac{2e^{ct}}{T} [\Im\{\bar{f}(c + i\omega_k)\} \sin \omega_k t]. \quad (7.4.22)$$

Note that (7.4.22) is similar to (7.4.4). Again, we let $h(t) = e^{-ct} f(t)$ and use the last two representations in (7.4.17) and (7.4.18). This yields

$$\sum_{n=0}^{\infty} e^{ct} k_n(t) = f(t) + \sum_{k=1}^{\infty} e^{-2ckT} [f(2kT + t) - e^{2ct} f(2kT - t)].$$

Thus, $f(t)$ can be represented as

$$f(t) + \text{Error}(E) = -\frac{2e^{ct}}{T} [\Im\{\bar{f}(c + i\omega_k)\} \sin \omega_k t]. \quad (7.4.23)$$

Adding (7.4.4) and (7.4.23) and dividing by 2, we get

$$\begin{aligned} f(t) + \frac{1}{2} (E_1 + E_2) \\ = \frac{e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \left\{ \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t \right. \right. \\ \left. \left. - \Im\{\bar{f}(c + i\omega_k)\} \sin \omega_k t \right\} \right], \end{aligned} \quad (7.4.24)$$

which can be compared with Crump's formula (7.4.13). The error E_2 in formula (7.4.24) is the average of the errors from (7.4.5) and (7.4.23), i.e.,

$$E_2 = \frac{1}{2} (E_1 + E_2) = \sum_{k=1}^{\infty} e^{-2ckT} f(2kT + t). \quad (7.4.25)$$

If $|f(t)| < C$, then

$$E_2 < \sum_{k=1}^{\infty} C e^{-2ckT} = \frac{C e^{-2cT}}{1 - e^{-2cT}} = \frac{C}{e^{2cT} - 1}. \quad (7.4.26)$$

Thus, the error estimate in (7.4.26) is superior since it does not depend on t , decreases as aT increases, and allows the representation (7.4.24) of $f(t)$ to be used for the interval $(0, T)$. If $|f(t)| \leq Ct^m$, then from (7.4.25) we find that

$$|E_2| \leq \sum_{k=1}^{\infty} C e^{-2ckT} (t + 2kT)^m \leq C (2T)^m \sum_{k=1}^{\infty} e^{-2ckT} (k+1)^m. \quad (7.4.27)$$

A comparison of the series on the right side of formula (7.4.27) to the integral $\int_1^{\infty} e^{-2cxT} (x+1)^m dx$ shows that the error E_2 is bounded by

$$|E_2| \leq A (2T)^m e^{-2cT} \sum_{k=1}^{m+1} \frac{\alpha_k}{(2cT)^k},$$

where A and α_k are constants (Durbin 1974).

Durbin's method is implemented as follows. First, take the average of formulas (7.4.6) and (7.4.23):

$$f(t) \approx \frac{e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t - \{\Im\{\bar{f}(c + i\omega_k)\} \sin \omega_k t\} \right], \quad (7.4.28)$$

and replace T by $T/2$ in formula (7.4.6) so that its applicability is extended to the interval $(0, 2T)$. But Kythe and Puri (2002) suggest to replace T by $2T$, and not by $T/2$, so as to cover the interval $(0, 2T)$. This leads to more accurate results. In fact, replacing T by $T/2$ in (7.4.6) and (7.4.28), we get Durbin's formulas (marked (41) and (42) in Durbin 1974):

$$\begin{aligned} f(t) &\approx \frac{4e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos 2\omega_k t \right] \\ f(t) &\approx \frac{2e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} \right. \\ &\quad \left. + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos 2\omega_k t - \{\Im\{\bar{f}(c + i\omega_k)\} \sin 2\omega_k t\} \right]. \end{aligned}$$

But if we replace T by $2T$ in (7.4.6) and (7.4.28), we get

$$\begin{aligned} f(t) &\approx \frac{e^{ct}}{T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t / 2 \right] \\ f(t) &\approx \frac{e^{ct}}{2T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} \right. \\ &\quad \left. + \sum_{k=1}^{\infty} \Re\{\bar{f}(c + i\omega_k)\} \cos \omega_k t / 2 - \{\Im\{\bar{f}(c + i\omega_k)\} \sin \omega_k t / 2\} \right], \end{aligned} \quad (7.4.29)$$

Both Dubner and Abate (1968) and Durbin (1974) suggest the use of the fast Laplace inverse transform (FLIT) for more efficient computation. Durbin's procedure for the FLIT is as follows: For $f(t)$ to be evaluated at equidistant points, set $t_j = j \Delta t$, where $\Delta t = jT/N$ for $j = 0, 1, 2, \dots, N-1$, define

$$s_k = c + 2i\omega_k, \quad \bar{f}(s_k) = \Re\{\bar{f}(s_k)\} + i\Im\{\bar{f}(s_k)\}. \quad (7.4.31)$$

This gives Durbin's formulas ((42) in Durbin 1974):

$$\begin{aligned} f(t) = E_2 + E_t + E_N &= \frac{e^{2cj\Delta t}}{2T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} \right. \\ &\quad \left. + \sum_{k=1}^N \Re\{\bar{f}(s_k)\} \cos \omega_k t_j / 2 - \{\Im\{\bar{f}(s_k)\} \sin 2\omega_k t_j\} \right], \end{aligned}$$

where Eq (7.4.31) is derived by replacing T by $T/2$. However, by the Kythe-Puri modification, the correct replacement is $2T$ in place of T , which yields

$$f(t) = E_2 + E_t + E_r$$

$$= \frac{e^{4cj\Delta t}}{2T} \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^N \Re\{\bar{f}(s_k)\} \cos 2\omega_k t_j - \{\Im\{\bar{f}(s_k)\} \sin 2\omega_k t_j\} \right], \quad (7.4.32)$$

where E_t and E_r represent the truncation and roundoff errors, respectively.

EXAMPLE 7.4.5. Consider Example 7.4.1, where $\bar{f}(s) = 1/(s^2 + s + 1)$. The values of $f(t)$ are presented in Table 7.4.5, which can be compared with those in Table 7.4.1. For computational details see [weeks.nb](#) on the CD-R. ■

Table 7.4.5.

t	Exact	Durbin	t	Exact	Durbin
0.0	0.000000	0.002026	5.5	0.039320	-0.073720
0.5	0.353907	0.377345	6.0	0.013679	-0.050895
1.0	0.403341	0.533507	6.5	-0.008259	-0.027236
1.5	0.245024	0.525425	7.0	-0.017710	-0.007647
2.0	0.034610	0.419279	7.5	-0.015174	0.005718
2.5	-0.109170	0.274111	8.0	-0.006552	0.012711
3.0	-0.145411	0.133242	8.5	0.001736	0.014516
3.5	-0.099507	0.022130	9.0	0.005953	0.012780
4.0	-0.025210	-0.049531	9.5	0.005731	0.009308
4.5	0.031623	-0.083450	10.0	0.002921	0.005380
5.0	0.051331	-0.087944			

EXAMPLE 7.4.6. (Durbin 1974) Consider $\bar{f}(s) = s(s^2 + 1)^{-2}$ for which $f(t) = 0.5t \sin t$. The results in Table 7.4.6 are computed for $N = 2000$ as well as for $N = 100, 500$, and 600 . The error appears at the fourth decimal digit for $N = 100$ and at the sixth decimal digit for both $N = 500$ and 600 . In this table f_1 (column 2) corresponds to Dubner and Abate's method (replacing T by $T/2$); f_2 (KP) (column 3) to Dubner and Abate's method (replacing T by $2T$); f_3 (column 4) to Durbin's (replacing T by $T/2$); f_4 (KP) (column 5) to Durbin's (replacing T by $2T$); column 6 to FLIT1 of Durbin (1974); column 7 to FLIT2 with T replaced by $2T$; and column 8 to the exact solution $f(t)$. All these results are obtained using Mathematica with $T = 20$, $aT = 5$, and $N = 2000$, where N is determined from the error estimates. It is obvious that the results in all cases where T is replaced by $2T$ are more accurate than those where T is replaced by $T/2$. Some of our results using Durbin's formula (42), in particular for $t = 1$, are different from those obtained by Durbin himself. For computational details, see [durbin.nb](#) on the CD-R. ■

Table 7.4.6.

t	f_1	f_2 (KP)	f_3	f_4 (KP)	FLIT1	FLIT2	Exact
0	0.1243	-1.2(-7)	0.0621	-6.1(-8)	0.0621	-6.1(-8)	0.0000
1	0.4970	0.4207	0.4797	0.4207	0.4797	0.4207	0.4207
2	0.7846	0.9092	0.9077	0.9092	0.9077	0.9092	0.9092
3	-0.1038	0.2116	0.1452	0.2116	0.1452	0.2116	0.2116
4	-1.7074	-1.5136	-1.5868	-1.5136	-1.5868	-1.5136	-1.5136
5	-2.0114	-2.3973	-2.4075	-2.3973	-2.4075	-2.3973	-2.3973
6	0.1760	-0.8382	-0.7705	-0.8382	-0.7705	-0.8382	-0.8382
7	3.0208	2.2994	2.3865	2.2994	2.3865	2.2994	2.2994
8	2.8200	3.9574	3.9821	3.9574	3.9821	3.9574	3.9574
9	-1.5723	1.8545	1.7886	1.8545	1.7886	1.8545	1.8545
10	-5.6405	-2.7201	-2.8202	-2.7201	-2.8202	-2.7201	-2.7201
11	-2.5924	-5.4999	-5.5413	-5.4999	-5.5413	-5.4999	-5.4999
12	7.6657	-3.2194	-3.1588	-3.2194	-3.1588	-3.2194	-3.2194
13	13.5386	2.7310	2.8427	2.7310	2.8427	2.7310	2.7310
14	1.3008	6.9342	6.9941	6.9342	6.9941	6.9342	6.9342
15	-24.5049	4.8772	4.8254	4.8771	4.8254	4.8771	4.8771
16	-34.2959	-2.3030	-2.4241	-2.3032	-2.4241	-2.3032	-2.3032
17	-3.4398	-8.1718	-8.2515	-8.1718	-8.2515	-8.1718	-8.1718
18	42.8424	-6.7592	-6.7196	-6.7588	-6.7196	-6.7588	-6.7588
19	44.7389	1.4230	1.5513	1.4238	1.5513	1.4238	1.4238

EXAMPLE 7.4.7. (Durbin 1974) Consider $\bar{f}(s) = \frac{e^{-10s}}{s}$ for which $f(t) = U(t - 10)$, where $U(x)$ is the unit step function. Table 7.4.7 presents the computed data for the same values of c, T , and N as in Example 7.4.6; the last five columns (2–6) represent the results obtained from formulas corresponding to those in Table 7.4.6, and the last column corresponds to the exact values of $f(t)$. Table 7.4.7 confirms the remarks made for Table 7.4.6. We have also found that Dubner and Abate’s formula (15) does not give the average value at the point of discontinuity when T is replaced by $T/2$, but it does yield the average value at the point of discontinuity when T is replaced by $2T$. For computational details, see `durbin.nb` on the CD-R. ■

EXAMPLE 7.4.8. (Durbin 1974) Consider $\bar{f}(s) = \frac{2}{s(1 + e^{-2s})}$ for which $f(t) = 2 \sum_{k=0}^\infty (-1)^k U(t - 2k)$, where $U(x)$ is the unit step function. Table 7.4.8 gives the values obtained from formula (7.4.29) in column 2; values obtained by Durbin (1974) using the FLIT in column 3; and the exact values in the last column. For computational details, see `durbin.nb` on the CD-R. We note that the accuracy of the two methods is about the same. ■

EXAMPLE 7.4.9. Consider $\bar{f}(s) = \frac{1}{s(1 + e^{-\pi s})}$, for which the exact solution

is the square wave with discontinuities at $t = n\pi$, where n is an integer, i.e., $f(t) = \sum_{n=0}^{\infty} (-1)^n U(t - n\pi)$, where $U(t - a)$ is the unit step function defined by $U(t - a) = 0$ for $t < a$, $U(t - a) = 0.5$ for $t = a$, and $U(t - a) = 1$ for $t > a$ (see [Abramowitz and Stegun 1968](#)).

Table 7.4.7.

t	f_1	f_2 (KP)	f_3	f_4 (KP)	Exact
0	0.01356	0.00003	0.00678	0.00001	0.0
1	0.01796	0.00004	0.00678	0.00002	0.0
2	0.02522	0.00005	0.00678	0.00003	0.0
3	0.03718	0.00007	0.00679	0.00005	0.0
4	0.05690	0.00010	0.00679	0.00007	0.0
5	0.08942	0.00014	0.00680	0.00011	0.0
6	0.14303	0.00022	0.00682	0.00018	0.0
7	0.23142	0.00036	0.00685	0.00031	0.0
8	0.37715	0.00067	0.00693	0.00061	0.0
9	0.61742	0.00164	0.00717	0.00157	0.0
10	1.01331	0.49957	0.50665	0.49949	0.5
11	1.01797	0.99749	1.00614	0.99740	1.0
12	1.02522	0.99844	1.00638	0.99833	1.0
13	1.03719	0.99871	1.00645	0.99857	1.0
14	1.05691	0.99879	1.00649	0.99863	1.0
15	1.08943	0.99879	1.00651	0.99860	1.0
16	1.14304	0.99874	1.00652	0.99852	1.0
17	1.23143	0.99864	1.00655	0.99838	1.0
18	1.37716	0.99850	1.00659	0.99819	1.0
19	1.61743	0.99833	1.00666	0.99795	1.0

Duffy (1993) has noted that many popular methods fail to provide a satisfactory result for this function because $\bar{f}(s)$ has infinitely many poles along the imaginary axis at $s = -(2n + 1)\pi i$, where n is an integer. We apply the modified Durbin's method (1974), and the results are presented in [Table 7.4.9](#). For computational details, see [ex7.4.8.nb](#) on the CD-R. ■

Albrecht and Honig (1977) use a min-max method and approximate $f(t)$ by

$$f_N(t) = \frac{e^{ct}}{T} \left[-\frac{1}{2} \Re \{ \bar{f}(c) \} + \sum_{k=1}^N (-1)^k \Re \left\{ \bar{f} \left(c + \frac{ik\pi}{T} \right) \right\} \right],$$

which is almost the same as in Durbin's formulation.

Table 7.4.8.

t	(7.4.29)	FLIT	Exact
0	0.99802	1.006615	1.0
1	1.99212	2.012790	2.0
2	0.99863	1.006321	1.0
3	0.00503	0.000511	0.0
4	0.99863	1.007322	1.0
5	1.99217	2.012833	2.0
6	0.99840	1.005719	1.0
7	0.00458	0.000549	0.0
8	0.99798	1.008010	1.0
9	1.99133	2.012913	2.0
10	0.99734	1.005268	1.0
11	0.00327	0.000820	0.0
12	0.99639	1.009086	1.0
13	1.98940	2.013551	2.0
14	0.99501	1.005602	1.0
15	0.00048	0.002814	0.0
16	0.99303	1.017248	1.0
17	1.98538	2.019597	2.0
18	0.99021	1.017248	1.0
19	-0.00525	0.039362	0.0

Table 7.4.9.

t	(7.4.29)	Exact	Error
0.0	0.506631	0.5	0.006631
1.0	1.00604	1.0	0.00604
$\pi/2$	1.0062	1.0	0.0062
2.0	0.999673	1.0	0.000327
3.0	0.997796	1.0	0.002204
π	0.500124	0.5	0.000124
4.0	0.000155	0.0	0.000155
5.0	-0.0000343	0.0	0.0000343
2π	0.507113	0.5	0.007113

7.4.4. Discretization Errors. All the above methods based on the Fourier series expansion approximate $f(t)$ by a truncated cosine, sine and complex Fourier series. We will denote expressions for $f(t)$ in these three cases by $f_1(t)$, $f_2(t)$ and

$f_3(t)$, respectively, so that for $t > 0$

$$\begin{aligned} f_1(t) &= \frac{2e^{ct}}{\pi} \int_0^\infty \Re\{\bar{f}(s)\} \cos \omega t \, d\omega, \\ f_2(t) &= -\frac{2e^{ct}}{\pi} \int_0^\infty \Im\{\bar{f}(s)\} \sin \omega t \, d\omega, \\ f_3(t) &= \frac{e^{ct}}{\pi} \int_0^\infty \Re\{\bar{f}(s) e^{i\omega t}\} \, d\omega, \end{aligned}$$

where f_1 and f_2 are contained in (7.4.1). After discretization of these three representations and using the trapezoidal rule with step size $h/\pi/T$, $t \in [0, T]$, we obtain $f_i(t) = \tilde{f}_i(t) + e_i$ for $i = 1, 2, 3$, where $\tilde{f}_1(t)$ is the right side of (7.4.6) or the real part in (7.4.7), $\tilde{f}_2(t)$ is the imaginary part with the minus sign of (7.4.7), and

$$\tilde{f}_3(t) = \frac{e^{ct}}{T} \Re\left\{\frac{1}{2} \bar{f}(c) + \sum_{k=1}^{\infty} \bar{f}(c + ik\pi/T) e^{ik\pi t/T}\right\},$$

with the discretization errors e_i , $i = 1, 2, 3$ which are defined by (de Hoog et al. 1982, D'Alessio et al. 1994)

$$\begin{aligned} e_1 &= \sum_{k=1}^{\infty} e^{-2ckT} \left\{ f(2kT + t) + e^{2ct} f(2kT - t) \right\}, \\ e_2 &= \sum_{k=1}^{\infty} e^{-2ckT} \left\{ f(2kT + t) - e^{2ct} f(2kT - t) \right\}, \\ e_3 &= \sum_{k=1}^{\infty} e^{-ckT} f(2kT + t), \end{aligned}$$

The methods of Dunbar and Abate (1968), Durbin (1974), Crump (1976), Honig and Hirdes (1984), and Piessens and Huysmans (1984) are based on the above analysis.

Let $s = c + iy$, $w = y + i\xi$, and $\gamma = c - c_0$. Murli and Patruno (1978) have proved that the functions

$$u(\gamma, w) = \frac{\bar{f}(\gamma + iw) - \bar{f}(\gamma - iw)}{2}, \quad v(\gamma, w) = \frac{\bar{f}(\gamma + iw) + \bar{f}(\gamma - iw)}{2i}$$

are analytic in the strip $|\xi| < \sigma$ in the complex w -plane, and that $u(c, y) = u(c, -y)$ and $v(c, y) = -v(c, -y)$. Define a class S_d of functions g for which $|g(s)| = |g(c + iy)| \leq A/|c|^\beta$ for $|c| \geq \delta$ and $|y| \leq d$ for all $A > 0$ and $\beta > 1$. Let $\bar{f}(s) = u(c, y) + i v(c, y)$ be the Laplace transform of a real function $f(t)$. If $u(\gamma, y) \in S_d$ and $t \in (0, \pi/2)$, then

$$f(t) \approx \frac{2h}{\pi} e^{\gamma t} \left[\frac{1}{2} u(\gamma, 0) + \sum_{k=1}^{\infty} u\left(\gamma, \frac{2\pi k}{\sigma t}\right) \cos \frac{2\pi k}{\sigma} \right], \quad (7.4.33a)$$

with the error bound

$$|e_1(t)| \leq \frac{4}{\pi} A M_1(d), \quad M_1(d) = \int_0^\infty |u(\gamma, y) + i d| dy, \quad (7.4.33b)$$

where $A = \frac{e^{-d(\sigma-1-\alpha)t}}{1 - e^{-d\sigma t}}$, and $d = \gamma/\alpha$, $\alpha > 1$, and $\sigma = 2\pi/(ht) > 2$. Similarly, using $v(c, y)$ instead of $u(c, y)$ we have the approximation

$$f(t) \approx -\frac{2h}{\pi} e^{\gamma t} \left[\frac{1}{2} u(\gamma, 0) + \sum_{k=1}^{\infty} u\left(\gamma, \frac{2\pi k}{\sigma t}\right) \sin \frac{2\pi k}{\sigma} \right], \quad (7.4.34a)$$

with the error bound

$$|e_2(t)| \leq \frac{4}{\pi} A M_2(d), \quad M_2(d) = \int_0^\infty |v(\gamma, y) + i d| dy, \quad (7.3.34b)$$

Note that the formulas (7.4.33) and (7.4.34) represent the approximations of the inverse Laplace transform, which use a series obtained by formally replacing the functions $\Re\{\bar{f}(s)\}$ and $\Im\{\bar{f}(s)\}$ by their Whittaker cardinal series, and the errors are defined in terms of $\bar{f}(s)$. Also, the integrand in $M_1(d)$ is $\Re\{\bar{f}(s)\}$, and that in $M_2(d)$ is $\Im\{\bar{f}(s)\}$. Thus, for the functions $f_i(t)$, $i = 1, 2, 3$ we have for $t > 0$ we get (D'Alessio et al. 1994)

$$\begin{aligned} f_1(t) &= \frac{e^{\gamma t}}{\pi} \int_{-\infty}^{\infty} u(\gamma, y) \cos ty dy + e_1(t), \\ f_2(t) &= -\frac{e^{\gamma t}}{\pi} \int_{-\infty}^{\infty} u(\gamma, y) \sin ty dy + e_2(t), \\ f_3(t) &= \frac{e^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} \Re\{\bar{f}(\gamma + i y) e^{ity}\} dy + e_3(t), \end{aligned} \quad (7.4.35)$$

where the corresponding truncation errors are

$$\begin{aligned} |e_1(t)| &\leq \frac{4}{\pi} A M_1(d), \\ |e_2(t)| &\leq \frac{4}{\pi} A M_2(d), \\ |e_e(t)| &\leq \frac{2}{\pi} A [M_1(d) + M_2(d)]. \end{aligned} \quad (7.4.36)$$

The error estimates (7.4.36) hold for any inversion formula derived from the Fourier series method, with the only restriction that $\bar{f}(s)$ be in the class S_d . The parameter γ , defined by $\gamma = c - c_0$ is another value of c ($> c_0$), and the parameter $\alpha > 1$ is arbitrary; Murli and Patruno (1978) take $\alpha = 1.1$. The value of σ is related to the discretization step size h by $\sigma = 2\pi/(ht)$, which by taking $h = \pi/T$ becomes

$\sigma = 2T/t$ and is easier to use because of its dependence on T which is known in advance.

7.4.5. Use of FFT Algorithm. Cooley et al. (1970) and Wing (1967) introduced the FFT algorithm to Weeks' method (§7.2.5(c)) to compute (7.2.21) for a_n in terms of the values of the left side of (7.2.21). There are two procedures for using the FFT technique to compute an inverse Fourier transform in terms of an expansion in terms of the Laguerre polynomials $L_n(x)$.

PROCEDURE 1. It starts with Weeks' method and goes through the following steps.

- (a) Select a scale factor T , a constant c , and an N , as defined in (7.2.23).
- (b) Let $\Delta\theta = 2\pi/N$, and $\theta_k = k \Delta\theta$ for $k = 0, 1, \dots, N-1$.
- (c) Compute $\eta_k = \frac{\pi}{2} \cot \frac{\theta_k}{2}$, $k = 0, 1, \dots, N-1$,
- (d) Compute the sequence $\{H_k\}_{k=0}^N = (i\eta_k + T/2) \bar{f}(c + i\eta_k)$.
- (e) Go to the FFT algorithm (§7.6.4) to compute

$$H_k = \sum_{j=0}^{N-1} h_j e^{2i\pi jk/N} \quad \text{for } k = 0, 1, \dots, N-1.$$

- (f) For each value at which the inverse Laplace transform $f(t)$ is desired, evaluate the series

$$f(t) \approx e^{(c-T/2)t} \sum_{j=0}^{N-1} h_j L_j\left(\frac{t}{T}\right), \quad (7.4.37)$$

which is the truncated series (7.2.19).

PROCEDURE 2. This is a direct application of Theorem 7.6.1. Consider $\bar{g}(s) = \int_0^\infty g(t) e^{-st} dt$. Let $s = c + i\eta$, where c and η are real. Then defining $\eta = 2\pi\omega$, we get

$$\bar{g}(s + 2i\pi\omega) = \int_0^\infty g(t) e^{-ct - 2i\pi\omega t} dt. \quad (7.4.38)$$

This Fourier transform pair contains the functions which are

$$F(\omega) = \bar{g}(c + 2i\pi\omega), \quad f(t) = U(t) g(t) e^{-ct}, \quad (7.4.39)$$

where $U(t)$ is the unit step function. There is one new positive parameter c in formula (7.4.38), which may be chosen by the user to optimize computation. There is a finite range of values of c that permit numerical accuracy. Substituting (7.4.39) into (7.4.38) we get $F(\omega)$ as the Fourier transform defined by $F(\omega) = \int_0^\infty f(t) e^{-2i\pi\omega t} dt$, with real and imaginary parts

$$\Re\{F(\omega)\} = \int_0^\infty f(t) \cos 2\pi\omega t dt, \quad \Im\{F(\omega)\} = \int_0^\infty f(t) \sin 2\pi\omega t dt. \quad (7.4.40)$$

We use Procedures 6 and 7 (§7.6.3) to compute the cosine and sine series for real data. The integrals in (7.4.40) can be written as complex integral transforms; thus,

$$\Re \{F(\omega)\} = \int_{-\infty}^{\infty} f_e(t) e^{-2i\pi\omega t} dt, \quad \Im \{F(\omega)\} = \int_{-\infty}^{\infty} f_o(t) e^{-2i\pi\omega t} dt,$$

where $f_e(t) = \frac{1}{2} [f(t) + f(-t)]$ and $f_o(t) = \frac{1}{2} [f(t) - f(-t)]$ are the even and odd parts of $f(t)$, respectively.

EXAMPLE 7.4.10. (Cooley et al. 1970) Consider the function $\bar{f}(s) = 1/s$, $s = c + i\eta$, $\eta = 2\pi\omega$. Then $\bar{f}(s) = \frac{c}{c^2 + (2\pi\omega)^2} - i \frac{2\pi\omega}{c^2 + (2\pi\omega)^2}$. Thus,

$$\Re \{F(\omega)\} = \frac{c}{c^2 + (2\pi\omega)^2}, \quad \Im \{F(\omega)\} = -i \frac{2\pi\omega}{c^2 + (2\pi\omega)^2}.$$

Since the periodized $F(\omega)$ is defined as $F_p(\omega) = \sum_{k=-\infty}^{\infty} F(\omega + k/\Delta t)$, the sum

$$\Re \{F_p(\omega)\} = \sum_{k=-\infty}^{\infty} \Re \{F(\omega + k/\Delta t)\} = \sum_{k=-\infty}^{\infty} \frac{c}{c^2 + (2\pi)^2(\omega + k/\Delta t)^2}$$

converges and is a real symmetric function of ω . Now, applying Theorem 7.6.1, the IDFT of the sequence $h_j = \Re \{F_p(j\Delta\omega)\}$ is the sequence $H_k = T f_{ep}(k\Delta t)$, where $f_{ep}(t) = \sum_{k=-\infty}^{\infty} f_e(t + kT)$ is the periodized $f_e(t)$.

The total error, due to aliasing and round-off, is

$$E = E_1 + E_2 = 2\hat{a}^{\tau/(T-\tau)} \hat{r}^{(T-2\tau)/(T-\tau)} = \begin{cases} 2\hat{r} & \text{at } \tau = 0, \\ 2\hat{a}^{1/3} \hat{r}^{2/3} & \text{at } \tau = T/4, \\ 2\hat{a} & \text{at } \tau = T/2, \end{cases}$$

where $\hat{a} = \max(T - t)$ and $\hat{r} = \max r(t)$, where the round-off error is given by $E_r = e^{ct} r(t)$, and $c = \frac{\ln(\bar{f}/\bar{r})}{T - \tau}$, $0 < t < \tau$. Thus, at $T/2$ the error is as large as $f(t)$ itself for all t . At smaller values of t , the error contains two factors: \bar{f} arising from aliasing, and \bar{r} arising from round-off. Therefore, the error criterion should be applied to a smaller range of t . The reasonable choice is to optimize the solution in the range $0 < t < T/4$, where we take c for $\tau = T/4$ as $c = \frac{4}{3T} \ln \frac{\bar{f}}{\bar{r}}$ to obtain an error less than $E = 2\bar{f}^{1/3}\bar{r}^{2/3}$.

For $\bar{f}(s) = 1/s$, $f(t) = U(t)$, and the IDFT gives the values of $H_k = T f_e(t_k) = \frac{T}{2} f(t_k)$. The error in $f(t)$ is bounded by $\bar{r} \leq \frac{2N}{T} 10^{-6} = \frac{2}{\Delta t} 10^{-6}$, with $T = 8$,

$N = 32$, which gives $\Delta t = 4$ and $\Delta\omega = 1/8$. Taking $\bar{f} = 1$, we get $\bar{r} = 8 \times 10^{-6}$, and the resulting error estimate is

$$E = 2(8 \times 10^{-6})^{2/3} = 8 \times 10^{-4},$$

with $c = \frac{4}{3T} \ln \frac{10^6}{8} = \frac{15.7}{T} \approx 2$ for $T = 8$. Thus, for this case we find computed values of $f(t)$ which are in the range $0 < t < T/4 = 2$ with error of at most 8 in the fourth digit. The limitation on the range seems to be the only drawback to this method. ■

EXAMPLE 7.4.11. (Cooley at al. 1970) The effect of the choice of c is displayed by carrying out the computations for the following transform pairs:

$$(i) \bar{f}(s) = \frac{e^{-4s}}{s} \longleftrightarrow f(t) = U(t - 4);$$

$$(ii) \bar{f}(s) = \frac{1}{\sqrt{s^2 + 1}} \longleftrightarrow f(t) = J_0(t);$$

$$(iii) \bar{f}(s) = \frac{1}{s^2} \longleftrightarrow f(t) = t.$$

All three cases are computed with $T = N = 32$, which gives the values $\Delta t = 1$, $1/\Delta = 1$, $\Delta\omega = 1/32$, so $\hat{r} = \frac{2}{\Delta t} \times 10^{-6} = 2 \times 10^{-6}$, and $\bar{f} = 1$; thus $c = \frac{4}{3T} \bar{f}^{1/3} \bar{r}^{2/3} = 2.6 \times 10^{-4}$. For example, for the case (ii) Cooley et al. (1970) have found the errors using $T = N = 32$ and $c = 0.3, 0.5, 0.7$, which are compared with those obtained by Durbin's method for $c = 0.3$. These results are presented in Table 7.4.11, which show a far better performance of Cooley et al. ■

Table 7.4.11. Errors in Example 7.4.11(ii).

		Cooley et al.		Durbin	
t	$f(t)$	$c = 0.3$	$c = 0.5$	$c = 0.3$	$c = 0.5$
0	1.00000000	15.1(−4)	25.4(−4)	5002.3(−4)	5004.0(−4)
1	0.76519789	0.0(−4)	0.1(−4)	10.9(−4)	13.3(−4)
2	0.22389078	0.2(−4)	0.1(−4)	7.3(−4)	10.8(−4)
3	−0.26005195	0.7(−4)	0.1(−4)	6.3(−4)	11.7(−4)
4	−0.39714981	0.5(−4)	0.1(−4)	6.4(−4)	14.1(−4)
5	−0.17759677	1.1(−4)	0.2(−4)	6.6(−4)	18.1(−4)
6	0.15064526	4.0(−4)	0.3(−4)	7.1(−4)	23.9(−4)
7	0.30007927	4.3(−4)	0.5(−4)	7.9(−4)	32.0(−4)
8	0.17165081	4.8(−4)	1.3(−4)	8.7(−4)	43.3(−4)

7.4.6. Improvement of the FFT Algorithm. (Hwang et al. 1991)

The method developed by Dunbar and Abate (1968), which uses the finite cosine transform, has the main drawback that the series (7.4.6) usually converges slowly and this formula is restricted to the interval $(0, T)$. Crump's method (1970) uses the complex Fourier series and develops the approximation (7.4.13) which we rewrite as

$$f(t) = \frac{e^{ct}}{2T} \sum_{k=-\infty}^{\infty} \bar{f}(c + ik\pi/T) e^{-ik\pi t/T}, \quad 0 < t < 2T. \quad (7.4.41)$$

Formula (7.4.41) is obtained after applying the trapezoidal rule with $\omega_k = k\pi/T$ and $\Delta\omega = \pi/T$. If we set $t = k\Delta t$ and $N\Delta T = 2T$ in (7.4.41), we obtain the approximation

$$f(k\Delta t) \approx \frac{e^{ck\Delta t}}{2T} \sum_{j=0}^{N-1} A_j e^{2i\pi jk/N}, \quad k = 0, 1, \dots, N-1, \quad (7.4.42a)$$

where

$$A_j = \sum_{n=-\infty}^{\infty} \bar{f}(c + i\pi(j + nN)/T), \quad (7.4.42b)$$

N is taken as radix 2, and the values of $f(k\Delta t)$ in (7.4.42) are computed by the FFT algorithm (§7.6.4). But this use of the FFT has the disadvantage of creating a compromise between the numerical accuracy and the computation effort. The interval of integration used in (7.4.41) is restricted to $\Delta\omega = \pi/T$, and a larger T is chosen for desired accuracy in cases where the function $\bar{f}(c + i\omega)$ is oscillatory. A larger value of T demands a larger value of N , which results in more computation time. Another drawback in formula (7.4.42) is that it produces an aliasing error (see [Examples 7.4.10](#) and [7.4.11](#) above).

Hwang et al. (1991) start with

$$f(t) = \frac{e^{ct}}{2\pi} \int_{-\infty}^{\infty} \bar{f}(c_i \omega) e^{i\omega t} d\omega \quad (7.4.43a)$$

$$= \frac{1}{\pi} \int_0^{\infty} \left[\Re \{ \bar{f}(c + i\omega) \} \cos \omega t - \Im \{ \bar{f}(c + i\omega) \} \sin \omega t \right] d\omega, \quad (7.4.43b)$$

and apply trapezoidal rule with $\omega = j\pi/(mT)$ and $\Delta\omega = \pi/(mT)$ to the integral (7.4.43a); then we obtain the complex Fourier series

$$\begin{aligned} f(t) &= \frac{e^{ct}}{2mT} \sum_{j=-\infty}^{\infty} \bar{f}(c + 2j\pi/(mT)) e^{i\pi jt/(mT)} \\ &= \frac{e^{ct}}{2mT} \sum_{j=-M}^M \bar{f}(c + 2j\pi/(mT)) e^{i\pi jt/(mT)} + e^{ct} E(t), \end{aligned} \quad (7.4.44)$$

where $E(t)$ is the truncation error. We choose a positive integer M such that $e^{ct} E(t)$ is negligibly small as compared to $|\tilde{f}(t)|$. Let $t = k\Delta T$, $\Delta T = 2T/N$, $M = \frac{mnN}{2} + \frac{m-1}{2}$, and taking N as radix 2, the FFT-based approximation, as developed by Hwang and Lu (1991), is

$$f(k\Delta T) = \frac{e^{ck\Delta t}}{2mT} \left(W^{N/2} \right)^{kn} \sum_{r=-m_1}^{m_2} \left\{ \sum_{j=0}^{N-1} \bar{f}_r(j) W^{jk} \right\}, \quad (7.4.45a)$$

$$= (-1)^{kn} \frac{e^{ck\Delta t}}{2mT} \sum_{r=-m_1}^{m_2} W^{kr/m} \left\{ \sum_{j=0}^{N-1} \bar{f}_r^*(j) W^{-jk} \right\}^*, \quad (7.4.45b)$$

where the asterisk denotes complex conjugate, and

$$m_1 = \left\lfloor \frac{m-1}{2} \right\rfloor, \text{ where } \lfloor \cdot \rfloor \text{ denotes the integral part,}$$

$$m_2 = \begin{cases} m_1 & \text{for } m \text{ odd,} \\ m_1 + 1 & \text{for } m \text{ even,} \end{cases}$$

$$\bar{f}_r(j) = \sum_{p=0}^{n_1} \bar{f}(c + i\pi(j + r/m + (2p-n)N/2)/T), \quad j = 0, 1, \dots, N-1, \quad (7.4.46)$$

$$n_1 = \begin{cases} n & \text{for } j = 0 \text{ and } r \neq m/2, \\ n-1 & \text{otherwise.} \end{cases}$$

Formula (7.4.45b), which is an improvement over FFT algorithm developed in §7.4.5 by Cooley et al. (1970), uses five parameters: c, T, N, m and n , where the values of $\tilde{f}(k\Delta T)$ for $k = 0, 1, \dots, N-1$, can be obtained by m sets of N -point FFT algorithm. With appropriate choices of these five parameters, the function $\bar{f}_r(j)$ can be computed from the given function $\tilde{f}(s)$ by using (7.4.46). Let

$$f_r(k) = \sum_{j=0}^{N-1} \bar{f}_r^*(j) W^{-jk}, \quad k = 0, 1, \dots, N-1, \quad (7.4.47)$$

and let the N -point sequences

$$\{\bar{f}_r^*(0), \bar{f}_r^*(1), \dots, \bar{f}_r^*(N-1)\} \quad \text{and} \quad \{f_r(0), f_r(1), \dots, f_r(N-1)\}$$

be denoted by $\{\bar{f}_r^*(j)\}_N$ and $\{f_r(k)\}_N$, respectively. Then the sequences $\{\bar{f}_r^*(j)\}_N$ become the output of the FFT subroutine with the sequence $\{f_r(k)\}_N$ as the input data, i.e.,

$$\{\bar{f}_r(k)\} \longleftrightarrow \{\bar{f}_r^*(j)\}_N.$$

The indicial function $f(t)$ at $t = k\Delta T$ is approximated by

$$f(k\Delta T) = (-1)^{kn} \frac{e^{ck\Delta T}}{2mT} \sum_{r=-m_1}^{m_2} f_r^*(k) W^{kr/m}, \quad k = 0, 1, \dots, N-1. \quad (7.4.48)$$

But formula (7.4.45b) need not actually perform m sets of N -point FFT computations because of the following relationships between $\bar{f}_r(j)$ and $\bar{f}_{-r}(j)$:

$$\begin{aligned} \bar{f}^*(c + i\omega) &= \bar{f}^*(c - i\omega), \\ \bar{f}_0(j) &= \begin{cases} \text{real} & \text{for } j = 0, N/2, \\ \bar{f}_0^*(N - j) & \text{for } j = 1, 2, \dots, N/2 - 1, \end{cases} \\ \bar{f}_r(j) &= \begin{cases} \bar{f}_{-r}^*(N - j) & \text{for } r = 1, 2, \dots, m_1, \\ \bar{f}^*(N - j - 1) & \text{for } j = 0, 1, \dots, N/2 - 1; r = m/2 \text{ and } m \text{ even.} \end{cases} \end{aligned} \quad (7.4.49)$$

Using these relations, formula (7.4.47) implies that the transformed sequences $\{f_r(k)\}$ have the following properties:

$$\begin{aligned} f_0(k) &\in R \quad \text{for } k = 0, 1, \dots, N-1, \\ f_r(k) &= f_{-r}^*(k) \quad \text{for } k = 0, 1, \dots, N-1, \\ \Im \{f_r^*(k) W^{k/2}\} &= 0 \quad \text{for } k = 1, \dots, N-1, r = m/2 \text{ and } m \text{ even.} \end{aligned} \quad (7.4.50)$$

Thus, we perform only $m_2 + 1$ sets of N -point FFT computations to compute $f(t)$ at $t = k\Delta T$ for $k = 0, 1, \dots, N-1$. Suppose the computed sequences are $\{f_r(j)\}_N$ at $r = 0, 1, \dots, m_2$. Then

$$f(k\Delta T) = (-1)^{kn} \frac{e^{ck\Delta T}}{2mT} \hat{f}(k), \quad (7.4.51)$$

where

$$\hat{f}(k) = \begin{cases} f_0(k) + 2 \sum_{r=1}^{m_1} \left[\Re \{f_r(k)\} \cos \frac{2\pi kr}{mN} - \Im \{f_r(k)\} \sin \frac{2\pi kr}{mN} \right] & \text{for } m \text{ odd,} \\ f_0(k) + 2 \sum_{r=1}^{m_1} \left[\Re \{f_r(k)\} \cos \frac{2\pi kr}{mN} - \Im \{f_r(k)\} \sin \frac{2\pi kr}{mN} \right] \\ \quad + \Re \{f_{m_2}(k)\} \frac{1}{\cos k\pi/N} & \text{for } m \text{ even.} \end{cases} \quad (7.4.52)$$

7.4.7. Use of the FHT Algorithm. (Hwang et al. 1991) Formula (7.4.45b) usually provides improved accuracy in computing the indicial function $f(t)$, but it also generates a faster FHT algorithm. From (6.7.2a,b) we note that the discrete Hartley pairs are given by

$$H(k) = \sum_{j=0}^{N-1} h(j) \operatorname{cas} \frac{2\pi jk}{N}, \quad h(j) = \frac{1}{N} \sum_{k=0}^{N-1} H(k) \operatorname{cas} \frac{2\pi jk}{N}.$$

Note that $H(k)$ and $h(j)$ are denoted by H_k and h_j in the DFT formulas. Let

$$H_r(k) = \sum_{j=0}^{N-1} h(j) \operatorname{cas} \frac{2\pi jk}{N},$$

and define the above transforms by the double-arrow relation

$$\{H_r(k)\}_N \longleftrightarrow \{h_r(j)\}_N, \quad r = -m_1, \dots, -1, 0, 1, \dots, m_2. \quad (7.4.53)$$

Let $\{H_r(k)\}_N$ be the output of the FHT subroutine with $\{h_r(j)\}_N$ as the input data:

$$\begin{aligned} H_r(k) &= \sum_{j=0}^{N-1} h_r(j) \operatorname{cas} \frac{2\pi jk}{N}, \quad k = 0, 1, \dots, N-1, \\ H_r(k) &= \Re\{f_r(k)\} + \Im\{f_r(N-k)\} \quad \text{for } k = 0, 1, \dots, N-1, \\ &\quad \text{and } r = -m_1, \dots, -1, 0, 1, \dots, m_2. \end{aligned}$$

Since $f_r^*(k) = f_{-r}(k)$, we get

$$\begin{aligned} H_0(k) &= f_0(k) \quad \text{for } k = 0, 1, \dots, N-1, \\ H_{-r}(k) &= \Re\{f_{-r}(k)\} + \Im\{f_{-r}(N-k)\} \\ &= \Re\{f_r(k)\} - \Im\{f_r(N-k)\} \quad \text{for } r = 1, 2, \dots, m_1, \end{aligned}$$

which gives

$$\begin{aligned} \Re\{f_r(k)\} &= \frac{1}{2} [H_r(k) + H_{-r}(k)], \\ \Im\{f_r(k)\} &= \frac{1}{2} [H_r(N-k) + H_{-r}(N-k)], \end{aligned}$$

for $k = 0, 1, \dots, N-1$ and $r = 0, 1, \dots, m_1$. Also,

$$W^{-k/2} f_{m/2}(k) = H_{m/2}(k) \cos \frac{k\pi}{N} + H_{m/2}(N-k) \sin \frac{k\pi}{N} \quad \text{for } m \text{ even.}$$

Thus, we have the approximation formula for $f(t)$ at $t = k\Delta T$, developed by Hwang et al. (1991):

$$\tilde{f}(k\Delta T) = \begin{cases} (-1)^k \frac{e^{ck\Delta T}}{2mT} \left[H_0(k) + \sum_{r=1}^{m_1} \left\{ [H_r(k) + H_{-r}(k)] \cos \frac{2\pi kr}{mN} \right. \right. \\ \quad \left. \left. - [H_r(N-k) + H_{-r}(N-k)] \sin \frac{2\pi kr}{mN} \right\} \right] & \text{for } m \text{ odd,} \\ (-1)^k \frac{e^{ck\Delta T}}{2mT} \left[H_0(k) + H_{m/2}(k) \cos \frac{k\pi}{N} - H_{m/2}(N-k) \sin \frac{k\pi}{N} \right. \\ \quad \left. + \sum_{r=1}^{m_1} \left\{ [H_r(k) + H_{-r}(k)] \cos \frac{2\pi kr}{mN} \right. \right. \\ \quad \left. \left. - [H_r(N-k) + H_{-r}(N-k)] \sin \frac{2\pi kr}{mN} \right\} \right] & \text{for } m \text{ even.} \end{cases} \quad (7.4.54)$$

This formula performs m sets of N -point real FHT computations as compared to formula (7.4.52) which performs $m_2 + 1$ sets of N -point FFT computations. Thus, formula (7.4.54) provides a significant reduction in computer time.

EXAMPLE 7.4.12. (Hwang et al. 1991) Consider three functions:

$$(i) f_1(s) = \frac{1}{s^2 + s + 1}, \quad f_1(t), \text{ for } c = -0.05;$$

$$(ii) f_2(s) = \frac{1}{(s + 0.2)^2 + 1}, \quad f_2(t) = e^{-0.2t} \sin t, \text{ for } c = 0.05;$$

$$(iii) f_3(s) = \frac{1}{(s + 1)^2}, \quad f_3(t) = t e^{-t}, \text{ for } c = -0.5;$$

$$(iv) f_4(s) = \frac{1}{s^2 + 1}, \quad f_4(t) = \sin t \text{ for } c = 0.2,$$

and compute the following two precision measures, which are modifications of those proposed by Davies and Martin (1979) (see §7.1) and defined by

$$L_1 = \sqrt{\sum_{j=0}^{63} \left(f(0.25j) - \tilde{f}(0.25j) \right)^2},$$

$$L_2 = \sqrt{\left(\sum_{j=0}^{63} \left(f(0.25j) - \tilde{f}(0.25j) \right) \right)^2 / \left(\sum_{j=0}^{63} e^{-0.25j} \right)},$$

where L_1 provides a fair test for successful computation for large t , and L_2 that for a relatively smaller t (compare L_1 and L_2 with L and L_e in (7.1.17) and (7.1.18)). These measures are computed for all these functions for $m = 1(1)4$ and $n = 1(1)8$. We present these values only for the case (ii) in Table 7.4.12; other results are available in Hwang et al. (1991). ■

The FFT method uses the time duration $T_{\max} = 2T$ to control the accuracy of the trapezoidal rule approximation (7.4.52), and thus it requires a large data set of complex FFT computations to obtain the function $f(t)$; sometimes it produces inaccurate results for $t > T_{\max}/2$. But the FHT formula (7.4.54) overcomes these disadvantages, since it takes a step size of $\Delta\omega = \pi/(mT)$ for the trapezoidal rule approximation which has an adjustable parameter m to control the order of precision, aliasing error, and computer cost.

D'Amore, Lacceti and Murli (1999b) have used the method based on the Fourier series expansion of $\tilde{f}(s)$ and produced a Fortran package INVLTF with subroutines QDACC and BACKCF, which uses the QD algorithm. This software is especially suitable when $\tilde{f}(s)$ is sectionally continuous. It is tested on $\tilde{f}(s) = 1/(s^2 + s + 1)$.

TABLE 7.4.12.

n	$m = 1$	$m = 2$	$m = 3$	$m = 4$
1	$L_1 = 0.74037(-2)$ $L_2 = 0.18549(-2)$	$0.61647(-3)$ $0.24925(-3)$	$0.58686(-3)$ $0.24789(-3)$	$0.60383(-3)$ $0.18085(-3)$
2	$L_1 = 0.72764(-2)$ $L_2 = 0.13962(-2)$	$0.20120(-3)$ $0.24346(-4)$	$0.91758(-4)$ $0.41904(-5)$	$0.92917(-4)$ $0.30473(-5)$
3	$L_1 = 0.73138(-2)$ $L_2 = 0.13794(-2)$	$0.14782(-3)$ $0.36570(-4)$	$0.49566(-4)$ $0.28310(-4)$	$0.53966(-4)$ $0.20625(-4)$
4	$L_1 = 0.73053(-2)$ $L_2 = 0.13764(-2)$	$0.14726(-3)$ $0.24276(-4)$	$0.12218(-4)$ $0.65629(-4)$	$0.13331(-4)$ $0.38485(-6)$
5	$L_1 = 0.73107(-2)$ $L_2 = 0.13765(-2)$	$0.14144(-3)$ $0.26006(-4)$	$0.17010(-4)$ $0.10281(-4)$	$0.18792(-4)$ $0.74696(-5)$
6	$L_1 = 0.73085(-2)$ $L_2 = 0.13758(-2)$	$0.14269(-3)$ $0.24264(-4)$	$0.36080(-5)$ $0.54188(-6)$	$0.40975(-5)$ $0.12153(-6)$
7	$L_1 = 0.73101(-2)$ $L_2 = 0.13760(-2)$	$0.14100(-3)$ $0.24657(-4)$	$0.89883(-5)$ $0.52832(-5)$	$0.95697(-5)$ $0.38213(-5)$
8	$L_1 = 0.73094(-2)$ $L_2 = 0.13757(-2)$	$0.14162(-3)$ $0.24270(-4)$	$0.24154(-5)$ $0.59861(-6)$	$0.17634(-5)$ $0.58828(-7)$

7.5. Use of Bromwich Contours

A Bromwich contour method is discussed for functions that have singularities.

7.5.1. Talbot's Method. Talbot (1979) uses the trapezoidal rule for the inversion of the Laplace transforms and computes the Bromwich integral (7.1.2) by computing it along a special contour which is defined below. The Bromwich contour in (7.1.2) from $c - i\infty$ to $c + i\infty$, where $c > c_0$, is chosen such that it is to the right of all singularities of $\bar{f}(s)$. However, the trapezoidal rule fails to give accurate results along the Bromwich contour because of the oscillations of e^{st} as $\Im\{s\} \rightarrow \pm\infty$. This difficulty was overcome by Levin (1975) who used his convergence-acceleration algorithms, although his method failed to achieve the error bounds of orders $O(10^{-12})$ to $O(10^{-15})$. Talbot's method circumvents this difficulty by changing the original Bromwich contour to a contour Γ in such a way that the trapezoidal rule becomes more accurate. The contour Γ starts and ends in the left half-plane so that $\Re\{s\} \rightarrow -\infty$ as $s \rightarrow c \pm i\infty$ and encloses all singularities of $\bar{f}(s)$ such that $\bar{f}(s) \rightarrow 0$ uniformly in $\Re\{s\} \leq c_0$ as $|s| \rightarrow \infty$. This method requires that (i) $\Im\{s\}$ remain bounded as $|s| \rightarrow \infty$ in order to limit the oscillations of e^{xs} , and (ii) $\Re\{s\} \rightarrow -\infty$ so that e^{xs} decays rapidly. In the case when the contour Γ does not enclose all singularities of $\bar{f}(s)$, we consider a modified function $\bar{f}(\lambda s + \sigma)$

by a suitable magnification parameter λ and a suitable translation σ ; then, if, for example, $\bar{f}(s)$ has a singularity at s_0 , then $\bar{f}(\lambda s + \sigma)$ will have this singularity at $s_0^* = (s_0 - \sigma)/\lambda$, and the integral (7.1.2) is replaced by

$$f(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_{\Gamma} e^{\lambda s t} \bar{f}(\lambda s + \sigma) ds, \quad t > 0. \quad (7.5.1)$$

In the particular case when $\bar{f}(s) = 1/s$, the contour Γ can be the steepest-descent contour for the integral (7.1.2) for $t > 0$. Then one can use the trapezoidal rule to evaluate this integral, using the parametric definition of the contour. In the general case, let M denote the imaginary interval $-2\pi i \leq s \leq 2\pi i$, and let $s = S(z)$ be a real uniform analytic function of $z = x + iy$ such that it (i) has simple poles at $\pm 2\pi i$, (ii) has no singularities in the strip $|y| < 2\pi$, (iii) maps the interval M one-to-one onto a contour Γ that is traversed upward in the s -plane such that Γ encloses all singularities of $\bar{f}(s)$ (or $\bar{f}(\lambda s + \sigma)$), and (iv) maps the half-strip $H : \{x > 0, |y| < 2\pi\}$ into the exterior of Γ . Then (7.5.1) can be written as

$$f(t) = \frac{1}{2\pi i} \int_M Q(z) dz = \frac{1}{2\pi} \int_{-2\pi}^{2\pi} Q(iy) dy, \quad (7.5.2)$$

where

$$Q(z) = \lambda e^{(\lambda S + \sigma)t} \bar{f}(\lambda S + \sigma) S'(z). \quad (7.5.3)$$

Note that in view of (i) and (ii), $\Re\{s\} \rightarrow \infty$ on Γ as $z \rightarrow \pm 2\pi i$ on M , and $Q(\pm 2\pi i) = 0$. Also, the condition (iii) depends on both \bar{f} and S but cannot be satisfied if $\bar{f}(s)$ has infinitely many singularities whose imaginary parts extend to infinity. These are the only kind of inverses $\bar{f}(s)$ which cannot be inverted by this method. Thus, excluding such functions $\bar{f}(s)$, we apply a trapezoidal rule to (7.5.1) and obtain the general approximate inversion formula:

$$\tilde{f}(t) = \frac{2}{n} \sum_{k=1}^{n-1} {}' \Re\{Q(z_k)\}, \quad \text{where } z_k = \frac{2k\pi i}{n}, \quad (7.5.4)$$

where $\tilde{f}(t)$ approximates the indicial function $f(t)$. Now, consider a family of mappings defined by $s = S_\nu(z) = \frac{z}{2} \left(\coth \frac{z}{2} + \nu \right) = \frac{z}{1 - e^{-z}} + az$, where $\nu > 0$ is an arbitrary parameter and $a = (\nu - 1)/2$. The singularities of $S_\nu(z)$ are the simple poles at $\pm 2n\pi i$, $n = 1, 2, \dots$. The function $S_\nu(z)$ maps the interval M onto a contour Γ_ν defined by

$$\Gamma_\nu : s = \sigma + \lambda s_\nu(\theta) = \sigma + \lambda(\alpha + i\nu\theta), \quad -\pi < \theta < \pi, \quad (7.5.5)$$

where $\alpha = \theta \cot \theta$. The contours Γ_ν are known as the *Talbot contours*, some of which are presented in Fig. 7.5.1 (see page 540), with the following legend: Γ_1 for

$\sigma = 1, \lambda = 1, \nu = 1; \Gamma_2$ for $\sigma = 2, \lambda = 1, \nu = 1; \Gamma_3$ for $\sigma = 1, \lambda = 1, \nu = 2$; and Γ_1 for $\sigma = 2, \lambda = 1, \nu = 2$.

On Γ_ν we have $S'_\nu(z) = s'_\nu(\theta) = (\nu + i\beta)/2$, where $\beta = \beta(\theta) = -d\alpha/d\theta = \theta + \alpha(\alpha - 1)\theta$. Then the approximation (7.5.4) becomes

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} \sum_{k=1}^{n-1} \Re \left\{ (\nu + i\beta) e^{s_\nu \tau} \bar{f}(\sigma + \lambda s_\nu) \right\}_{\theta=\theta_k}, \quad (7.5.6)$$

where $\tau = \lambda t$, and $\theta_k = k\pi/n$, $k = 0, 1, \dots, n-1$. If $\bar{f}(\sigma + \lambda s_\nu) = G + iH$, then (7.5.6) takes the real form

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} \sum_{k=1}^{n-1} \left[e^{\alpha t} \left\{ (\nu G - \beta H) \cos(\nu\theta\tau) - (\nu H + \beta G) \sin(\nu\theta\tau) \right\} \right]_{\theta=\theta_k}. \quad (7.5.7)$$

The error in this formula is given by $E(t) = E_1(t) + E_2(t)$, where $E_1 = f(t) - \tilde{f}(t)$ is the theoretical error and has a bound of order $O\left(n^2 e^{ht-b\sqrt{n}\tau+\sigma t}\right)$, and h and b are constants. Talbot (1979) has shown that both $E_{1,2} \rightarrow 0$ as $n \rightarrow \infty$. The predicted error in the formula (7.5.7) is then given by

$$T_0 = \frac{\lambda}{n} e^{(\lambda S(0)+\sigma)t} \bar{f}(\lambda S(0) + \sigma) S'(0), \quad (7.5.8)$$

If the computer evaluates T_0 correct to d significant digits, the round-off error E_r in \tilde{f} is approximately $E_r = (10^{-d} T_0)$, and all other round-off errors are negligible in its comparison. Hence, the actual error in \tilde{f} is $E = E_1 + E_2 + E_r \approx O(10^{-d} T_0)$ for sufficiently large n . Talbot (1979) has considered a set of twenty cases of Laplace inverses, which are given in Table 7.5.1.

An implementation of this method is given in Murli and Rizzardi (1990) where two computer routines are available. Given the points x where the Laplace transform is to be inverted, the locations and types of the singularities of \bar{f} , and the desired accuracy, the first routine computes the parameters σ , λ , and ν , while the second routine applies the trapezoidal rule using n points which are equally spaced. The contour is parametrized by $s(\theta) = \sigma + \lambda s_\nu(\theta)$, $\theta \in (-\pi, \pi)$, where $s_\nu(\theta) = \theta \cot \theta + i\nu\theta$. Then formula (7.5.1) becomes

$$f(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_{-\pi}^{\pi} e^{\lambda t s_\nu(\theta)} \bar{f}(\sigma + \lambda s_\nu(\theta)) s'_\nu(\theta) d\theta, \\ s'_\nu(\theta) = i \left\{ \nu + \frac{\theta - \cos \theta \sin \theta}{\sin^2 \theta} \right\}. \quad (7.5.9)$$

Using symmetry, the trapezoidal rule approximation gives

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} T_n(t), \\ T_n(t) = \sum_{j=1}^n e^{\lambda t s_\nu(\theta_j)} \bar{f}(\sigma + \lambda s_\nu(\theta_j)) \frac{1}{i} s'_\nu(\theta_j), \quad \theta_j = \frac{j\pi}{n}. \quad (7.5.10)$$

Table 7.5.1.

$\bar{f}(s)$	$f(t)$
1. $\frac{1}{\sqrt{s^2-1}}$	$I_0(t)$
2. $\frac{e^{-s/\sqrt{s+1}}}{s}$	—
3. $e^{-\sqrt{s}}$	$\frac{1}{2\sqrt{\pi t^3}} \exp\left(-\frac{1}{4t}\right)$
4. $\frac{1}{(s+1)^5}$	$\frac{t^4 e^{-t}}{24}$
5. $\frac{999}{(s+1)(s+1000)}$	$e^{-t} - e^{-1000t}$
6. $-\frac{\gamma_e + \ln s}{s}$	$\ln t, \quad \gamma_e = 0.5772156649$
7. $\frac{2}{\sqrt{s} + \sqrt{s+1}}$	$\frac{1 - e^{-t}}{\sqrt{\pi t^3}}$
8. $\frac{e^{-1/s}}{\sqrt{s}}$	$\frac{\cos 2\sqrt{t}}{\sqrt{\pi t}}$
9. $\tan^{-1}\left(\frac{1}{s}\right)$	$\frac{\sin t}{t}$
10. $\frac{1}{\sqrt{s^2+1}}$	$J_0(t)$
11. $\frac{1}{\sqrt{s + \sqrt{s^2+1}}}$	$\frac{\sin t}{\sqrt{2\pi t^3}}$
12. $\frac{\sqrt{s + \sqrt{s^2+1}}}{\sqrt{s^2+1}}$	$\sqrt{\frac{2}{\pi t}} \sin t$
13. $\frac{(s + \sqrt{s^2+1})^{3/2}}{\sqrt{s^2+1}}$	$\sqrt{\frac{2}{\pi t^3}} (\sin t - \cos t)$
14. $\frac{\sqrt{s + \sqrt{s^2+1}} e^{s-\sqrt{s^2+1}}}{\sqrt{s^2+1}}$	$\sqrt{\frac{2}{\pi(t+2)}} \sin \sqrt{t(t+2)}$
15. $\frac{s}{(s^2+1)\sqrt{s+1}}$	—
16. $\frac{s^3}{s^4+4}$	$\cos t \cosh t$
17. $\frac{1}{s^4-1}$	$\frac{\sinh t - \sin t}{2}$
18. $\frac{1}{(s^2+1)^2}$	$\frac{\sin t - t \cos t}{2}$
19. $\frac{s^2}{s^3+8}$	$\frac{e^{-2t} - 2 \cos(\sqrt{3}t) e^t}{3}$
20. $\ln\left(\frac{s^2+1}{s^2+4}\right)$	$\frac{2(\cos 2t - \cos t)}{t}$

In the sum (7.5.10), the $j = n$ term is zero and the $j = 0$ term is $\frac{\nu}{2} e^{\lambda t} \bar{f}(\sigma + \lambda)$. Talbot (1979) uses the following values: $\lambda = \frac{\omega - 1}{t} + \frac{1}{30}$, $\omega = 0.4(d + 1)$, where d denotes the decimal machine precision. But Murli and Rizzardi (1990) use $\lambda = \frac{\omega - 1}{t} + \frac{1}{\sqrt{\omega t}}$ with the same value of ω as in Talbot's case. The procedure overflows when $t > 10^3$. They increase n to $n' = n \log_2(t)$ when $t > 10$. With this modification their result is correct for $t < 10^5$. For large t the overflow problem remains, but it can be mitigated by increasing λ . Since Murli and Rizzardi's software is available, we will not discuss it further.

Rizzardi (1995) has generalized Talbot's method to approximate simultaneously several values of $f(t)$ using the same sampling values of the Laplace transform. This method eliminates the only unfavorable aspect of Talbot's method, which consists in recomputing the values of $\bar{f}(s)$ for each t . The test functions used are: $\bar{f}_1(s) = 1/s^2$, $\bar{f}_2(s) = 1/(s - 1)$, $\bar{f}_3(s) = \arctan(1/s)$, and $\bar{f}_4(s) = s^2/(s^3 + 8)$.

7.5.2. Duffy's Method. Duffy (1993) has tested the following three methods on complicated transform function: (i) Trapezoidal rule, (ii) Weeks' method using Laguerre polynomials, and (iii) the classical Talbot's method. The test functions are:

1. $\bar{f}(s) = \frac{1}{s(s + c)} \left[\frac{1}{2hs} - \frac{e^{-2hs}}{1 - e^{-2hs}} \right]$, where c and h are real parameters. The inverse is given by

$$f(t) = \frac{1}{2c} + \frac{e^{-ct}}{c} \left[\frac{1}{2hc} - \frac{e^{2hc}}{e^{2hc} - 1} \right] - \frac{h}{\pi} \sum_{n=1}^{\infty} \frac{\sin \left[\frac{n\pi t}{h} - \arctan \left(\frac{n\pi}{hc} \right) \right]}{n \sqrt{n^2 \pi^2 + h^2 c^2}}.$$

This inverse arises in circuit theory (McLachlan 1953, §8.63).

2. $\bar{f}(s) = \frac{(100s - 1) \sinh(\sqrt{s}/2)}{s [s \sinh \sqrt{s} + \sqrt{s} \cosh \sqrt{s}]}$, which has poles on the negative real axis at $s = -b_n^2$, where $b_n \tan b_n = 1$. The inverse is given by

$$f(t) = -\frac{1}{2} + \sum_{n=1}^{\infty} \left(100 + \frac{1}{b_n^2} \right) \frac{2b_n \sin(b_n/2) e^{-b_n^2 t}}{(2 + b_n^2) \cos b_n}.$$

This inverse is encountered in the study of longitudinal impact on viscoplastic rods (Ting and Symonds 1964).

3. $\bar{f}(s) = \frac{1}{s} e^{-a\sqrt{s(1+s)/(1+cs)}}$, which has the inverse

$$f(t) = \frac{1}{2} + \frac{1}{\pi} \int_0^{\infty} e^{-am\sqrt{m/2} (\cos \theta - \sin \theta)} \times \sin \left[tu - am\sqrt{u/2} (\cos \theta + \sin \theta) \right] \frac{du}{u},$$

where $m = \left(\frac{1+u^2}{1+c^2u^2} \right)^{1/4}$ and $2\theta = \arctan(u) - \arctan(cu)$. This function arises in the Rayleigh problem for a viscoelastic fluid (Tanner 1962).

4. $\bar{f}(s) = \frac{e^{-2\Psi}}{s}$, where $\cosh \Psi = \sqrt{1+s^2+s^2/16}$. The function $f(t)$ is given by

$$f(t) = 1 - \frac{1}{\pi} \int_0^{u_1} \left[\sin(ut + 2k) - \sin(ut - 2k) \right] \frac{du}{u} \\ + \frac{1}{\pi} \int_{u_2}^4 \left[\sin(ut + 2k) - \sin(ut - 2k) \right] \frac{du}{u},$$

where $\cos k = \frac{1}{4} \sqrt{(u_1^2 - u^2)(u_2^2 - u^2)}$, and $u_{1,2} = 2\sqrt{2 \mp \sqrt{3}}$. This function appears in the study of shock waves in diatomic chains (Musgrave and Tasi 1976).

5. $\bar{f}(s) = \frac{s - \sqrt{s^2 - c^2}}{\sqrt{s} \sqrt{s^2 - c^2} \sqrt{s - N} \sqrt{s^2 - c^2}}$, $N < 1$, which gives

$$f(t) = \frac{2}{\pi} \int_0^c \cosh(tu) \frac{u \sqrt{(R+u)/2} + \sqrt{c^2 - u^2} \sqrt{(R-u)/2}}{R \sqrt{c^2 - u^2} \sqrt{u}} \\ + \frac{2}{\pi} \int_0^b \frac{u - \sqrt{c^2 + u^2}}{\sqrt{u} \sqrt{c^2 + u^2} \sqrt{N} \sqrt{(c^2 + u^2) - u}} \cos(tu) du,$$

where $R = \sqrt{(u^2 + N^2 \sqrt{c^2 - u^2})}$, $b = \sqrt{(1-N)/(1+N)}$, and $c = (1-N)/N$. This function arises in the theory of beams (Boley and Chao 1955). A couple of joint Fourier-Laplace transforms are also discussed.

7.6. Inversion by the Riemann Sum

(Tzou, Özisik and Chiffelle 1994, and Tzou 1997) Assuming that the real number c in definition (7.1.2) of the inverse $f(t)$ is taken to the right of all singularities of $\bar{f}(s)$, and substituting $s = c + i\omega$, we can write

$$\frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} \bar{f}(s) e^{st} ds = \frac{e^{ct}}{2\pi} \int_{-\infty}^{\infty} \bar{f}(c + i\omega) e^{i\omega t} d\omega. \quad (7.6.1)$$

Replacing ω by $\frac{n\pi}{\tau}$ and $\Delta\omega_n$ by π/τ , the integral on the right side of (7.6.1) can be

expressed as a Riemann sum:

$$\begin{aligned}
 \frac{e^{ct}}{2\pi} \int_{-\infty}^{\infty} \bar{f}(c+i\omega) e^{i\omega t} d\omega &= \frac{e^{ct}}{2\tau} \sum_{n=-\infty}^{\infty} \bar{f}\left(c + \frac{in\pi}{\tau}\right) e^{in\pi t/\tau} \\
 &= \frac{e^{ct}}{2\tau} \left[\bar{f}(c) + \sum_{n=1}^{\infty} \left[\bar{f}\left(c + \frac{in\pi}{\tau}\right) e^{in\pi t/\tau} + \bar{f}\left(c - \frac{in\pi}{\tau}\right) e^{-in\pi t/\tau} \right] \right] \\
 &= \frac{e^{ct}}{\tau} \left[\frac{1}{2} \bar{f}(c) + \Re \left\{ \sum_{n=1}^{\infty} \bar{f}\left(c + \frac{in\pi}{\tau}\right) e^{in\pi t/\tau} \right\} \right].
 \end{aligned} \tag{7.6.2}$$

Then for $\tau = t$, we get

$$f(t) = \frac{e^{ct}}{t} \left[\frac{1}{2} \bar{f}(a) + \Re \left\{ \sum_{n=1}^{\infty} (-1)^n \bar{f}\left(c + \frac{in\pi}{t}\right) \right\} \right]. \tag{7.6.3}$$

Thus, integration is reduced to an infinite series. The accuracy of formula (7.6.3), which was also given by Crump (1976), depends on the choice of c and N . Note that formula (7.6.2) is equivalent to formula (7.4.28). According to Tzou et al. (1994) and Tzou (1997), the best choice for c appears to be $4.7/t$. The disadvantage, as Crump (1976) points out, is that one has to choose a different c for each t . But this can be remedied by replacing ct by b and changing formula (7.6.3) to

$$f(t) = \frac{e^b}{t} \left[\frac{1}{2} \bar{f}\left(\frac{b}{t}\right) + \Re \left\{ \sum_{n=1}^{\infty} (-1)^n \bar{f}\left(\frac{b}{t} + \frac{in\pi}{t}\right) \right\} \right]. \tag{7.6.4}$$

Also note that formulas (7.6.4) and (7.4.32) are closely related.

EXAMPLE 7.6.1. Consider $f(t) = 0.5t \sin t$, for which $\bar{f}(s) = \frac{s}{s^2 + 1}$; and $f(t) = U(t-10)$, for which $\bar{f}(s) = \frac{e^{-10s}}{s}$. The values of approximate $f(t)$ obtained from formula (7.6.4) are given in [Table 7.6.1](#). There is no change in these values for $n = 1000$ or 10000 . Since formula (7.6.4) has singularity at $t = 0$, we have evaluated $\tilde{f}(t)$ at $t = 0.0001$. For computational details see [tzou.nb](#) on the CD-R. ■

EXAMPLE 7.6.2. Jordan et al. (2000) have used this method to compute the following two inverses:

$$\bar{f}_1(s) = -\frac{2}{\pi} \int_0^1 g(u, x, t) dt, \quad \bar{f}_2(s) = e^{-x/b} - 1 + \int_0^1 h(u, x, t) du,$$

where

$$g(u, x, t) = \frac{u e^{-tu^2/(1-u)^2} \sin[xj(u)]}{(1-u)\sqrt{(1-u)^4 + 2u^2(2b^2 - a^2)(1-u)^2 + a^4u^4}},$$

$$h(u, x, t) = \frac{(1-u) e^{-tu^2/(1-u)^2} \sin[xj(u)]}{(1-u)\sqrt{(1-u)^4 + 2u^2(2b^2 = a^2)(1-u)^2 + a^4u^4}},$$
$$j(u) = \frac{1}{b(1-u)} \times \sqrt{\frac{a^2u^2 - (1-u^2) + \sqrt{(1-u)^4 + 2u^2(2b^2 - a^2)(1-u)^2 + a^4u^4}}{2}}. \blacksquare$$

Table 7.6.1.

t	$0.5\,t\sin t$	(7.6.4)	$U(t-10)$	(7.6.4)
0	0.00000	5.00372(−9)	0.0	0.00000
1	0.42073	0.42075	0.0	3.87(−21)
2	0.90929	0.90922	0.0	3.41(−9)
3	0.21168	0.21183	0.0	6.83(−9)
4	−1.51360	−1.51387	0.0	8.25(−5)
5	−2.39731	−2.39691	0.0	8.27(−5)
6	−0.83824	−0.83880	0.0	7.47(−5)
7	2.29945	2.30018	0.0	5.61(−5)
8	3.95743	3.95653	0.0	0.00020
9	1.85453	1.85560	0.0	−0.00003
10	−2.72011	−2.72133	0.5	0.49960
11	−5.49995	−5.49858	1.0	1.00178
12	−3.21944	−3.22091	1.0	1.00103
13	2.73109	2.73264	1.0	1.00132
14	6.93425	6.93266	1.0	0.99881
15	4.87716	4.87874	1.0	1.00008
16	−2.30323	−2.30475	1.0	1.00147
17	−8.17188	−8.17046	1.0	0.99826
18	−6.75889	−6.76013	1.0	1.00108
19	1.42383	1.42486	1.0	0.99797

7.7. New Exact Laplace Inverse Transforms

Since the publication of tables of Laplace inversion formulas published in Erdélyi et al. (1954), Roberts and Kaufman (1966), Abramowitz and Stegun (1968), Oberhettinger and Badu (1973), and others, some new exact inversion formulas have been published

in research journals. An attempt has been made to collect all such formulas and present them as the file `NewLaplaceInverses.pdf` which is available on the CD-R. These new formulas are taken from the work of Hetnarski (1964, 1975), Gridamo (1974), Puri and Kulshrestha (1974), Puri (1984), Puri and Kythe (1988), Jordon, Puri and Boros (2000), and Jordan, Meyer and Puri (2000). This pdf file may not be complete. In that case the readers are encouraged to point out the publications where we have missed other exact new inversion formulas. We will present such new formulas on our website and acknowledge the individuals for their contribution.

8

Wavelets

To some extent wavelets are no more different than other orthogonal systems. They are an extension of Fourier analysis and used to represent a function by a series of orthogonal functions, but with these differences: The wavelet series converge pointwise, are more localized, exhibit edge effects better, and use fewer coefficients to represent certain signals and images. However, wavelet expansions undergo excessive changes under arbitrary translations, which makes the situation much worse than the Fourier series. We study wavelets in the same manner as in the previous chapters with other orthogonal systems, in particular with orthogonal polynomials and Fourier series. Wavelets are computed by fast transforms.

Orthogonal series have been used since their inception and Fourier provided the trigonometric Fourier series to solve partial differential equations of heat conduction and wave propagation. Orthogonal polynomials, like Legendre and Hermite, are used in solving the Laplace and Schrödinger equations. They have been extensively used in Gaussian quadrature. We will study the unique properties of the orthogonal (and orthonormal) sequences of wavelets and their transforms.

8.1. Orthogonal Systems

A nontrivial sequence $\{f_n\}_{n=0}^{\infty}$ of real (or complex) functions in $L_2(a, b)$ is said to be *orthogonal* if $\langle f_n, f_m \rangle = \int_a^b f_n(x) f_m^*(x) dx = 0$ for $n \neq m$, where $n, m = 0, 1, 2, \dots$, and *orthonormal* if in addition $\langle f_n, f_n \rangle = 1$ for $n = 0, 1, 2, \dots$.

EXAMPLE 8.1.1. The sequence $\{f_n\} = \{\sin(n+1)x\}$ is orthogonal on $(0, \pi)$. ■

EXAMPLE 8.1.2. The sequence $\{f_n(x)\}$, where

$$f_n = \chi_{[n, n+1)}(x) = \begin{cases} 1, & n \leq x < n+1, \\ 0, & \text{elsewhere,} \end{cases}$$

is orthonormal on $[0, \infty)$. ■

Given a function $f(x) \in L_2(a, b)$, we seek to expand it in an orthonormal series

$$f(x) = \sum_{n=0}^{\infty} c_n f_n(x). \quad (8.1.1)$$

If this is possible, the coefficients c_n must have a special form (this is not always the case is obvious if we take $f(x) = \chi_{[1/2, 1)}(x)$ in Example 8.1.2). In fact, let $\{c_n\}$ be a sequence such that the series (8.1.1) converges to $f(x)$ in the L_2 -norm, defined by $\|f\|_2 = \langle f, f \rangle^{1/2}$. Then $c_n = \langle f, f_n \rangle$, and the mean-square error is given by $E_n = \|f - \sum_{n=0}^N c_n f_n\|$. The expansion (8.1.1) is always possible if c_n are Fourier coefficients. Thus, if $\{c_n\}$ is the sequence of Fourier coefficients of $f \in L_2(a, b)$ and if $\{a_n\}$ is any other sequence, then $\|f - \sum_{n=0}^{\infty} c_n f_n\|^2 \leq \|f - \sum_{n=0}^{\infty} a_n f_n\|^2$; i.e., the mean-square error is a minimum for the series with Fourier coefficients. We can also say that the Fourier coefficients give the orthogonal projection of f onto the subspace V_n spanned by (f_0, f_1, \dots, f_N) , and $\langle \sum_{n=0}^N c_n f_n, f - \sum_{n=0}^N c_n f_n \rangle = 0$; i.e., the best approximation to f in V_N is given by this sum, and the error E_n is orthogonal to V_N . Moreover, the orthonormal system $\{f_n\}$ is said to be *complete* in $L_2(a, b)$ if no nontrivial $f \in L_2(a, b)$ is orthogonal to all f_n ; i.e., $\langle f, f_n \rangle = 0, n = 0, 1, 2, \dots$ implies that $f = 0$ almost everywhere. Thus, if $\{f_n\}$ is an orthonormal system in $L_2(a, b)$, and if the expansion of $f \in L_2(a, b)$ has the Fourier coefficients $\{c_n\}$, then $\|f - \sum_{n=0}^N c_n f_n\| \rightarrow 0$ as $N \rightarrow \infty$ iff $\{f_n\}$ is complete.

For any orthonormal system $\{f_n\}$, we have Bessel's inequality

$$\sum_k |c_k|^2 \leq \|f\|_2^2, \quad (8.1.2)$$

where equality occurs if the system is a basis for $L_2(R)$. Conversely, if an orthonormal system $\{f_n\}$ satisfies the condition

$$\sum_k |c_k|^2 = \|f\|_2^2, \quad (8.1.3)$$

for all $f \in L_2(R)$, then the system is a basis for $L_2(R)$. We will discuss some orthonormal systems in detail in the following sections.

8.2. Trigonometric System

This system, defined by $f_0(x) = \frac{1}{2}$, $f_1(x) = \sin x$, $f_2(x) = \cos x, \dots, f_{2n-1}(x) = \sin nx$, $f_{2n}(x) = \cos nx, \dots$, is a complete orthogonal system in $L_2(-\pi, \pi)$, but it is not orthonormal since $\|f_n\|^2 = \pi$ for $n \neq 0$. The trigonometric series is written as

$$s(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx), \quad (8.2.1)$$

and if the series $s(x)$ is the Fourier series of a function $f \in L_2(-\pi, \pi)$, then the coefficients a_n and b_n are given by

$$\begin{aligned} a_0 &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx, & a_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx dx, \\ b_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx dx, & n &= 1, 2, \dots \end{aligned}$$

Let $s_n(x) = \frac{a_0}{2} + \sum_{k=1}^n (a_k \cos kx + b_k \sin kx)$ denote the partial sum of the Fourier series for f . If f is a 2π -periodic function in $C^2(R)$, then $\sup_{x \in R} |s_n(x) - f(x)| \rightarrow 0$ and $\|s_n - f\| \rightarrow 0$ as $n \rightarrow \infty$; i.e., the series $s(x)$ converges uniformly to a limit function f which is 2π -periodic and continuous. The Fourier series (8.2.1) for a $2P$ -periodic function f becomes

$$f(x) = A_0 + \sum_{n=1}^{\infty} \left(A_n \cos \frac{n\pi x}{P} + B_n \sin \frac{n\pi x}{P} \right), \quad (8.2.2)$$

where

$$\begin{aligned} A_0 &= \frac{1}{2P} \int_{-P}^P f(x) dx, & A_n &= \frac{1}{P} \int_{-P}^P f(x) \cos \frac{n\pi x}{P} dx, \\ B_n &= \frac{1}{P} \int_{-P}^P f(x) \sin \frac{n\pi x}{P} dx, & n &= 1, 2, \dots \end{aligned}$$

The *Dirichlet kernel* $D_n(u)$ is defined by

$$D_n(u) = \frac{1}{\pi} \left[\frac{1}{2} + \sum_{k=1}^n \cos ku \right] = \frac{\sin(n + 1/2)u}{2\pi \sin(u/2)}, \quad (8.2.3)$$

and is such that $\int_{-\pi}^{\pi} D_n(u) du = 1$.

If f is piecewise continuous on every finite interval and $\int_{-\infty}^{\infty} |f(x)| dx < \infty$, then f has the Fourier integral representation

$$f(x) = \int_0^{\infty} [A(\gamma) \cos \gamma x + B(\gamma) \sin \gamma x] d\gamma, \quad -\infty < x < \infty, \quad (8.2.4)$$

where for all $\gamma \geq 0$

$$A(\gamma) = \frac{1}{\pi} \int_{-\infty}^{\infty} f(x) \cos \gamma t dt, \quad B(\gamma) = \frac{1}{\pi} \int_{-\infty}^{\infty} f(x) \sin \gamma t dt. \quad (8.2.5)$$

The integral in (8.2.4) converges to $f(x)$ if f is continuous and to $\frac{1}{2} [f(x+) + f(x-)]$ otherwise. Note the similarity between the Fourier integral (8.1.5) and the Fourier series (8.2.2). Suppose that f is integrable on the real line, and we restrict f to a finite interval $(-P, P)$. We take the part of f that is inside $(-P, P)$ and extend its periodicity outside this interval. This periodic extension agrees with f on $(-P, P)$ and has the Fourier series (8.2.2), which represents $f(x)$ for $x \in (-P, P)$. Then what happens to this representation as $P \rightarrow \infty$? To answer this question, we examine the Fourier coefficients as $P \rightarrow \infty$. Since f is integrable, it follows that $A_0 \rightarrow 0$ as $P \rightarrow \infty$. Also, a relationship between A_n, B_n and $A(\gamma), B(\gamma)$, respectively, can be established as follows. The integrability of f implies that the integrals in (8.2.4) can be approximated by integrating over the (large) finite interval $(-P, P)$. The difference is just the tail ends of the integrals, which can be made arbitrarily small. Thus, by (8.2.5) for large P we have

$$A_n \approx \frac{1}{P} \int_{-P}^P f(x) \cos \frac{n\pi x}{P} dx = A(\gamma_n) \Delta\gamma,$$

where $\gamma_n = n\pi/P$ and $\Delta\gamma = \pi/P$. Similarly, $B_n \approx B(\gamma_n) \Delta\gamma$. Substituting these values in (8.2.2) we find that for very large P

$$f(x) = \sum_{n=1}^{\infty} [A(\gamma_n) \cos \gamma_n x + B(\gamma_n) \sin \gamma_n x] \Delta\gamma. \quad (8.2.6)$$

The sum in (8.2.6) is a Riemann sum, which samples the integrands of (8.2.5) at equally spaced points γ_n with a partition size $\Delta\gamma$ which is exactly the distance between two consecutive γ_n . Since $n \rightarrow \infty$ in (8.2.6), the Riemann sum in (8.2.6) is not taken over a finite interval but spans the entire nonnegative γ -axis regardless of P . Then as $P \rightarrow \infty$, we have $\Delta\gamma \rightarrow 0$ and this Riemann sum converges to the integral given by (8.2.4).

EXAMPLE 8.2.1. To find the Fourier representation of the function

$$f(x) = \begin{cases} 1 & \text{if } |x| < 1, \\ 0 & \text{otherwise,} \end{cases}$$

note that $A(\gamma) = \frac{2 \sin \gamma}{\pi \gamma}$, $B(\gamma) = 0$ (since f is even), and for $|x| \neq 1$ we get

$$f(x) = \frac{2}{\pi} \int_0^\infty \frac{\sin \gamma \cos \gamma x}{\gamma} d\gamma.$$

For $x = \pm 1$, which are the points of discontinuity of f , we obtain the value $\frac{1}{2}$. Hence,

$$f(x) = \frac{2}{\pi} \int_0^\infty \frac{\sin \gamma \cos \gamma x}{\gamma} d\gamma = \begin{cases} 1 & \text{if } |x| < 1, \\ \frac{1}{2} & \text{if } |x| = 1, \\ 0 & \text{if } |x| > 1. \end{cases}$$

If we set $x = 0$ in the above integral representation of f , we obtain the Dirichlet integral $\int_0^\infty \frac{\sin \gamma}{\gamma} d\gamma = \frac{\pi}{2}$, which is a special case of (8.2.3). ■

Let the partial Fourier integral of f be denoted by

$$S_n(x) = \int_0^n [A(\gamma) \cos \gamma x + B(\gamma) \sin \gamma x] d\gamma, \quad n > 0, \quad (8.2.7)$$

where $A(\gamma)$ and $B(\gamma)$ are given by (8.2.5). Then $\lim_{n \rightarrow \infty} S_n(x) = \frac{1}{2} [f(x+) + f(x-)]$. The Fourier integral, like the Fourier series, exhibits a *Gibbs phenomenon* near a point of discontinuity. We introduce the sine integral function

$$\text{Si}(x) = \int_0^\infty \frac{\sin t}{t} dt, \quad -\infty < x < \infty.$$

Then $\lim_{x \rightarrow \infty} \text{Si}(x) = \pi/2$.

EXAMPLE 8.2.2. The partial Fourier integral for the function $f(x)$ in Example 8.2.1 is given by

$$\begin{aligned} S_n(x) &= \frac{2}{\pi} \int_0^n \frac{\sin \gamma \cos \gamma x}{\gamma} d\gamma \\ &= \frac{1}{\pi} \int_0^n \left\{ \frac{\sin \gamma(1+x)}{\gamma} + \frac{\sin \gamma(1-x)}{\gamma} \right\} d\gamma \\ &= \frac{1}{\pi} \left[\int_0^{n(1+x)} \frac{\sin u}{u} du + \int_0^{n(1-x)} \frac{\sin u}{u} du \right] \\ &= \frac{1}{\pi} [\text{Si}(n(1+x)) + \text{Si}(n(1-x))]. \end{aligned} \quad (8.2.8)$$

The graphs of $S_n(x)$ for $n = 1, 4, 6, 8, 10$ are given in Fig. 8.2.1 (see page 541), where the Gibbs phenomenon at the point of discontinuity of f is exhibited by the overshooting of the graphs beyond their limiting values. ■

LITTLEWOOD-PALEY THEOREM. (Littlewood and Paley 1931,1936) Using the Fourier series $f(x) = a_0 + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx)$, we define the ‘dyadic blocks’ $\Delta_j f(x)$ by

$$\Delta_j f(x) = \sum_{2^j < k < 2^{j+1}} (a_k \cos kx + b_k \sin kx). \quad (8.2.9)$$

Then $f(x) = a_0 + \sum_{j=0}^{\infty} \Delta_j f(x)$. Littlewood and Paley (1936) prove that there exist two constants $C_p \geq c_p > 0$ for $1 < p < \infty$ such that

$$c_p \|f_p\| \leq \left\| \left(|a_0|^2 + \sum_{j=0}^{\infty} |\Delta_j f(x)|^2 \right)^{1/2} \right\|_p \leq C_p \|f\|_p. \quad (8.2.10)$$

This result is sharp for $p = 2$ and $C_p = c_p = 1$.

8.3. Haar System

In the sequel the letters j, k, l, m, n, p and r denote integers. To discuss the Haar orthogonal system we first consider the interval $[0, 1)$ and start with the characteristic function of the unit interval

$$\phi(t) = \chi_{[0,1)}(t), \quad (8.3.1)$$

which is known as the *scaling function* of the Haar wavelet (Haar 1910) defined by

$$\psi(t) = \begin{cases} 1, & 0 \leq t < 1/2, \\ -1, & 1/2 \leq t < 1, \\ 0, & \text{outside } [0, 1), \end{cases} \quad (8.3.2)$$

such that $\int_{-\infty}^{\infty} \psi(t) dt = 0$ and $\|\psi(t)\|^2 = \int_{-\infty}^{\infty} |\psi(t)|^2 dt = 1$. The function $\psi(t)$ is also known as the *mother wavelet* of the Haar family; it is localized in the time domain but is not continuous. The father and mother wavelets are related by $\psi(t) = \phi(2t) - \phi(2t - 1)$. The first generations of the daughter wavelets are

$$\psi_{10}(t) = \psi(2t), \quad \text{and} \quad \psi_{11}(t) = \psi(2t - 1),$$

and they are related to the father wavelet by

$$\psi_{10}(t) = \phi(4t) - \phi(4t - 1), \quad \psi_{11}(t) = \phi(4t - 2) - \phi(4t - 3). \quad (8.3.3)$$

The plots of $\phi(t)$, $\psi(t)$, $\psi_{10}(t)$, and $\psi_{11}(t)$ are given in Fig. 8.3.1 (see page 541). Note that $\chi_{[0,b)}(t) = \chi_{[0,1)}(t/b)$, and $\chi_{[a,b)}(t) = \chi_{[0,1)}\left(\frac{t-a}{b-a}\right)$. We will sometimes use the following notation:

$$\phi_k^{(n-m)}(t) = \phi_{[0,1)}(2^{n-m}t - k) = \begin{cases} 1 & \text{if } k2^{m-n} \leq t < (k+1)2^{m-n}, \\ 0 & \text{elsewhere,} \end{cases} \quad (8.3.4)$$

$$\psi_k^{(n-m)}(t) = \psi_{[0,1)}(2^{n-m}t - k) = \begin{cases} 1 & \text{if } k2^{m-n} \leq t < (k + \frac{1}{2})2^{m-n}, \\ -1 & \text{if } (k + \frac{1}{2})2^{m-n} \leq t < (k+1)2^{m-n}, \\ 0 & \text{elsewhere.} \end{cases} \quad (8.3.5)$$

Let V_n denote the set of all functions that are constant on the intervals of the form $\left[\frac{m}{2^n}, \frac{m+1}{2^n}\right)$ of length 2^{-n} , where $m = 0, 1, \dots, 2^n - 1$, and zero elsewhere. The set V_n is also an inner product vector space of functions $f(t)$ with a finite norm $\|f\| = \sqrt{\langle f, f \rangle}$. In particular, V_0 is the set of all functions that are constant on the interval $[0, 1)$, and zero elsewhere; V_1 is the set of all functions that are constant on the ‘halves’, i.e., on the intervals $[0, 1/2)$ and $[1/2, 1)$, and zero outside the interval $[0, 1)$; V_2 is the set of all functions that are constant on the ‘quarters’, i.e., on the intervals $[0, 1/4)$, $[1/4, 1/2)$, $[1/2, 3/4)$, $[3/4, 1)$, and zero outside the interval $[0, 1)$. Then there is a 1–1 correspondence between V_0 and R , between V_1 and R^2 , between V_2 and R^4 , and so on. For example, the correspondence between V_2 and R^4 is given by

$$f(t) = \begin{cases} a, & 0 \leq t < 1/4, \\ b, & 1/4 \leq t < 1/2, \\ c, & 1/2 \leq t < 3/4, \\ d, & 3/4 \leq t < 1, \\ 0, & \text{elsewhere.} \end{cases} \longleftrightarrow \begin{Bmatrix} a \\ b \\ c \\ d \end{Bmatrix}. \quad (8.3.6)$$

Thus, we can write

$$\phi \longleftrightarrow \begin{Bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{Bmatrix}, \quad \psi \longleftrightarrow \begin{Bmatrix} 1 \\ 1 \\ -1 \\ 1 \end{Bmatrix}, \quad \psi_{10} \longleftrightarrow \begin{Bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{Bmatrix}, \quad \psi_{11} \longleftrightarrow \begin{Bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{Bmatrix}. \quad (8.3.7)$$

For example, in the case of ψ_{11} the matrix representation means that it has the first-element value 0 in the interval $[0, 1/4)$, the second-element value 0 in $[1/4, 1/2)$, the third-element value 1 in $[1/2, 3/4)$, and the fourth-element value -1 in $[3/4, 1)$.

The *second generation daughters*, related to the set V_3 , are

$$\begin{aligned} \psi_{20}(t) &= \psi(4t), & \psi_{22}(t) &= \psi(4t - 2), \\ \psi_{21}(t) &= \psi(4t - 1), & \psi_{23}(t) &= \psi(4t - 3). \end{aligned} \quad (8.3.8)$$

The wavelets are ‘constant on the eighths’ (i.e., intervals of length $1/8$), and a relationship of the type (8.3.6) between V_3 and R^8 can be easily established. For the plots of the wavelets (8.3.8), see Fig. 8.3.2 (see page 542). In general, for each positive integer n , the n -th generation of daughters has 2^n wavelets, defined by

$$\psi_{nk}(t) = \psi(2^n t - k), \quad 0 \leq k \leq 2^j - 1, \quad (8.3.9)$$

and there is a 1–1 correspondence between V_n and R^{2^n} .

In view of (8.3.7) we can also denote the father wavelet $\phi(t)$ as $\phi_{[0,1)}(t)$, the mother wavelet as $\psi_{[0,1)}(t)$, and the first generation daughter wavelets as $\psi_{10}(t) = \psi_{[0,1/2)}(t)$ and $\psi_{11}(t) = \psi_{[1/2,1)}(t)$. Similarly, in view of (8.3.5) the second generation daughter wavelets are represented as

$$\begin{aligned} \psi_{20}(t) &= \psi(4t) = \psi_{[0,1/4)}(t), & \psi_{22}(t) &= \psi(4t - 2) = \psi_{[1/2,3/4)}(t), \\ \psi_{21}(t) &= \psi(4t - 1) = \psi_{[1/4,1/2)}(t), & \psi_{23}(t) &= \psi(4t - 3) = \psi_{[3/4,1)}(t). \end{aligned}$$

Let W denote a finite-dimensional subspace of V , and W^\perp the orthogonal complement of $W \neq \emptyset$ (also called the annihilator), i.e., $W^\perp = \{\mathbf{v} \in V : \langle \mathbf{v}, \mathbf{w} \rangle = 0 \text{ for all } \mathbf{w} \in W\}$ (see Kreyszig 1978, p. 148). Then the *orthogonal decomposition theorem* states that any $\mathbf{v} \in V$ can be uniquely written as $\mathbf{v} = \mathbf{w} + \mathbf{w}_\perp$, where $\mathbf{w} \in W$ and $\mathbf{w}_\perp \in W^\perp$, i.e., $V = W \oplus W^\perp$, and

$$\mathbf{w} = \sum_{k=1}^n \frac{\langle \mathbf{v}, \mathbf{w}_k \rangle}{\langle \mathbf{w}_k, \mathbf{w}_k \rangle}. \quad (8.3.10)$$

The vector \mathbf{w} is called the *orthogonal projection* of V onto W , and the vector \mathbf{w}_\perp the *residual*.

EXAMPLE 8.3.1. Using the basis

$$B_2 = \{\phi, \psi, \psi_{10}, \psi_{11}\} = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & -1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & -1 & 0 & -1 \end{bmatrix}, \quad (8.3.11)$$

the orthogonal projection of $f(t) = t$ onto V_2 is

$$f(t) = \frac{1}{2} \phi(t) = \frac{1}{4} \psi(t) - \frac{1}{8} \psi_{10}(t) - \frac{1}{8} \psi_{11}(t).$$

Also, $\langle \psi_{10}(t), \psi_{11}(t) \rangle = 0$, which means that $\psi_{10} \perp \psi_{11}$. Note that B_2 is a basis for R^4 (or V_2). ■

The standard basis in R^4 is

$$S_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (8.3.12)$$

The columns of this basis contain the functions ϕ_{20} , ϕ_{21} , ϕ_{22} , and ϕ_{23} , respectively, which are defined by

$$\begin{aligned}\phi_{20}(t) &= \psi(2^2 t), & \phi_{22}(t) &= \psi(2^2 t - 2), \\ \phi_{21}(t) &= \psi(2^2 t - 1), & \phi_{23}(t) &= \psi(2^2 t - 3).\end{aligned}\quad (8.3.13)$$

These functions are known as the *second generations of wavelet sons*. Their graphs are given in Fig. 8.3.3 (see page 542). In general, for each positive integer n , the n -th generation of wavelet boys are defined by

$$\phi_{n,k}(t) = \phi(2^n t - k), \quad 0 \leq k \leq 2^n - 1. \quad (8.3.14)$$

Note that in view of (8.3.4) the second generation son wavelets can be represented as

$$\begin{aligned}\phi_{20}(t) &= \phi(4t) = \phi_{[0,1/4)}(t), & \phi_{22}(t) &= \phi(4t - 2) = \phi_{[1/2,3/4)}(t), \\ \phi_{21}(t) &= \phi(4t - 1) = \phi_{[1/4,1/2)}(t), & \phi_{23}(t) &= \phi(4t - 3) = \phi_{[3/4,1)}(t).\end{aligned}$$

For a given n , the set S_n denotes the set of 2^n functions $\{\phi_{nk}(t)\}_{k=0}^{2^n-1}$. The set S_n forms a basis for the inner product space V_n . The father wavelet $\phi(t)$ satisfies the *dilation property*:

$$\phi(t) = \sum_{k=-\infty}^{\infty} c_k \phi(2t - k). \quad (8.3.15)$$

For the Haar wavelet, the coefficients $c_0 = c_1 = 1$ and $c_j = 0$ for $j \neq 0, 1$. The projection of $\phi_{11}(t)$ onto V_0 is $\frac{1}{2} \phi(t)$, and $\phi_{20}(t) = \frac{1}{4} \phi(t) + \frac{1}{4} \psi(t) + \frac{1}{2} \psi_{10}(t)$.

EXAMPLE 8.3.2. We will write functions $f(t)$ that belong to V_2 as a linear combination of the father, mother and the first generation of daughter wavelets. Consider a function $f(t)$ defined by

$$f(t) = \begin{cases} 4 & \text{if } t \in [0, 1/4), \\ -1 & \text{if } t \in [1/4, 1/2), \\ 1 & \text{if } t \in [1/2, 3/4), \\ -9 & \text{if } t \in [3/4, 1), \\ 0 & \text{elsewhere.} \end{cases}$$

Thus, we determine the coefficients $\mathbf{x} = [x_1, x_2, x_3, x_4]^T$ such that

$$f(t) = x_1 \phi(t) + x_2 \psi(t) + x_3 \psi_{10}(t) + x_4 \psi_{11}(t). \quad (8.3.16)$$

Since there is a 1 – 1 correspondence between V_2 and R^4 , we can write Eq (8.3.16) in the matrix form as

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & -1 & 0 & 1 \\ 1 & -1 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} 4 \\ -1 \\ 1 \\ -9 \end{Bmatrix},$$

which is solved to yield $[x_1 \ x_2 \ x_3 \ x_4]^T = [5/4 \ 1/4 \ -13/4 \ 23/4]^T$. The plot of $f(t)$ is given in Fig. 8.3.4 (see page 543). ■

In this example the vector \mathbf{b} forms the signal $f(t)$ and the elements of the vector \mathbf{x} are called the *wavelet coefficients*. The process of solving the equation $\mathbf{A}\mathbf{x} = \mathbf{b}$ is known as the decomposition of a signal into wavelet coefficients; the reverse process where the vector \mathbf{x} is known and the vector \mathbf{b} is to be computed is known as the recomposition of a signal from its wavelet coefficients. The (square) matrix is known as the (Haar) wavelet matrix for $n = 2$. This process can be easily generalized to involve the father, mother, and j -generation of daughter wavelets for $j = 1, 2, \dots, n$. Since B_2 is a basis for R^4 , we always obtain a unique solution for Eq (8.3.16); i.e., every $f \in V_2$ can be uniquely expressed as a linear combination of ϕ, ψ, ψ_{10} , and ψ_{11} . This is also true for V_n .

Since $V_0 \subseteq V_1$, then by the orthogonal decomposition theorem each function $h \in V_1$ can be written as $f + g$, where $f \in V_0$ and $g \in V_0^\perp$, i.e., $V_1 = V_0 \oplus V_0^\perp$.

EXAMPLE 8.3.3. The projection of $\phi_{10} \in S_1$ onto V_0 is

$$\frac{\langle \phi_{10}, \phi \rangle}{\langle \phi, \phi \rangle} = \frac{1}{2} \phi. \quad (8.3.17)$$

The residual which is the projection of ϕ_{10} onto V_0^\perp is given by $\phi_{10} - \frac{1}{2} \phi = \frac{1}{2} \psi$. ■

The space V_0^\perp is one-dimensional, because $\dim(V_1) = 2$ and $\dim(V_0) = 1$. The residuals of both ϕ_{10} and ϕ_{11} are scalar multiples of ψ . Hence, $\{\psi\}$, which arises from S_1 , is a basis for V_0^\perp . In fact, $\psi \in V_1$ and ψ is orthogonal to all elements of V_0 . Thus, we obtain another basis for V_1 . Since $S_0 = \{\phi\}$ is a basis for V_0 and $C_0 = \{\psi\}$ is a basis for V_0^\perp , then by the orthogonal decomposition theorem $B_1 = S_0 \cup C_0 = \{\psi, \phi\}$ is a basis for V_1 . Similarly, $C_1 = \{\psi_{1k}\}$, where $\psi_{1k}(t) = \psi(2t - k)$, $k = 0, 1$, is a basis for V_1^\perp . Continuing this construction to n , since $V_n \subseteq V_{n+1}$, we get $V_{n+1} = V_n \oplus V_n^\perp$, and this creates a basis C_n of V_n^\perp , given by $C_n = \{\psi_{nk}\}$, where $\psi_{nk}(t) = \psi(2^n t - k)$, $k = 0, 1, \dots, 2^n - 1$. Then $B_{n+1} = B_n \cup C_n$ is a basis for V_{n+1} . In general,

$$\begin{aligned} V_n &= V_{n+1} \oplus V_{n-1}^\perp = \left(V_{n-2} \oplus V_{n-2}^\perp \right) \oplus V_{n-1}^\perp \\ &= \dots = V_0 \oplus V_0^\perp \oplus V_1^\perp \oplus \dots \oplus V_{n-1}^\perp. \end{aligned} \quad (8.3.18)$$

Thus, B_n is obtained from the standard basis S_n , and B_n provides the wavelet coefficients in the general cases involving the parent and daughter wavelets.

8.3.1. Extension to the Real Axis. We will enlarge the Haar system by including functions of the form $\phi(2^j t)$. Then the sequence $\{\phi(t - n)\}$, defined on the dyadic intervals $I_{j,k} = [k 2^j, (k + 1) 2^j)$ of length 2^j , where a larger value of j means longer intervals $I_{j,k}$ and the corresponding wavelet functions $\psi_{jk}(t)$ represent longer ‘waves’, is not a complete orthogonal system in $L_2(R)$, since the closed linear

system V_0 contains piecewise constant functions with jump discontinuities at the integer points. Then a basis for V_0 is $\{\phi(t - k)\}$. Similarly, the space V_1 consists of piecewise constant functions with compact support with discontinuities at the rational points which are midway between the integers, and V_2 similar functions with compact support and discontinuities at rational points with denominators 2^{-2} . In general, the space V_n contains piecewise constant functions with compact support and discontinuities at the rational points of the form $m \times 2^{-n}$ for any integer m . For negative n the discontinuities become far removed from each other. Thus, a basis for V_n is $\{\phi(2^n t - k)\}$. The norm of a function $f \in V_n$ is $\|f\| = \langle f, f \rangle^{1/2} = \left(\int_{-\infty}^{\infty} [f(t)]^2 dt \right)^{1/2} < \infty$.

The scaling function $\phi(t) = \chi_{[0,1/2)}(t)$ cannot have a convergent expansion of the form (8.1.1). We will enlarge this system by including more functions of the form $\phi(2^j t)$. Then the sequence $\{\phi_{jk}(t)\} = \{2^{j/2} \phi(2^j t - k)\}$ becomes an orthonormal system with its closed linear span V_j . The system $\{\phi_{jk}\}$ is also complete in $L_2(R)$, but since $\phi(t)$ and $\phi(2t)$ are not orthogonal, it is not an orthogonal system. But if we set $\psi(t) = \phi(2t) - \phi(2t - 1)$, then $\{\psi(t - k)\}$ becomes an orthogonal system, and $\psi(2t - k)$ and $\psi(t - n)$ are orthogonal for all k and n . Thus, the system $\{\psi_{jk}(t)\}$, where $\psi_{jk}(t) = 2^{j/2} \psi(2^j t - k)$, is a complete orthonormal system in $L_2(R)$. The amplitude of $\psi_{j,k}(t)$ is chosen such that $\|\psi_{j,k}(t)\|^2 = \int_{-\infty}^{\infty} |\psi_{j,k}(t)|^2 dt = 1$ for all j and k . Thus, the functions $\psi_{j,k}(t)$ form an orthonormal basis of the space $L_2(R)$ (also known as the Haar basis), such that $\langle \psi_{j,k}, \psi_{j,m} \rangle = 0$ for $k \neq m$ and $\langle \psi_{j,k}, \psi_{l,m} \rangle = 0$ for $j \neq l$ and all k and m . A constructive proof of this result is available in Blatter (1998, pp. 22–25), which can be summarized as follows. Define a signal $f \in L_2$ such that $f(t) \equiv 0$ for $|t| \geq 2^m$, $m \geq 0$, and f is a step function which is constant on the intervals $I_{-n,k}$ of length 2^{-n} , $n \geq 0$. Then a sequence of wavelet polynomials $\{\Psi_r\}$, $r \geq -n$, is constructed from the wavelet functions $\psi_{j,k}$ by

$$\Psi_r = \sum_{j=-n+1}^r \left(\sum_k c_{j,k} \psi_{j,k} \right), \quad (8.3.19)$$

such that $f = \Psi_r + f_r$, where f_r is the remainder after the r terms, and f_r is constant on each interval $I_{j,k}$. In this construction we start with $\Psi_{-n} = 0$, $f_{-n} = f$, and using recursion on r ($r \rightarrow r + 1$), we define

$$\delta_{r',k} = \frac{1}{2} [f_{r,2k} - f_{r,2k+1}], \quad f_{r',k} = \frac{1}{2} [f_{r,2k} + f_{r,2k+1}].$$

Let

$$c_{r',k} = 2^{r'/2} \delta_{r',k}, \quad \Psi_{r'} = \Psi_r + \sum_k c_{r',k} \psi_{r',k}, \quad f_{r'}(t) = f_{r',k}, \quad t \in I_{r',k}. \quad (8.3.20)$$

In the recursion we begin with $r = -n$. Then after $n + m$ steps we get

$$f = \Psi_m + f_m = \sum_{j=-n+1}^m \left(\sum_k c_{j,k} \psi_{j,k} \right) + f_m. \quad (8.3.21)$$

The remainder f_m in (8.3.21) is constant on the intervals $I_{m,k}$ of length 2^m , and $f_{m,-1} \neq 0$ and $f_{m,0} \neq 0$, where $f_{m,-1}$ is the value of f on $[-2^m, 0)$ and $f_{m,0}$ is the value of f on $[0, 2^m)$. After additional p steps we obtain

$$f_m = \sum_{j=m+1}^{m+p} \left(\sum_k c_{j,k} \psi_{j,k} \right) + f_{m+p},$$

where the function f_{m+p} is constant on the interval $[-2^{m+p}, 0) \cup (0, 2^{m+p}]$ and zero outside it. Since $f \equiv 0$ outside the interval $[-2^m, 2^m)$, we get

$$f_{m+p,-1} = 2^{-p} f_{m,-1}, \quad f_{m+p,0} = 2^{-p} f_{m,0}.$$

Thus,

$$\|f_{m+p}\|^2 = \int_{-\infty}^{\infty} |f_{m+p}(t)|^2 dt = 2^{m+p} \left[2^{-2p} |f_{m,-1}|^2 + 2^{-2p} |f_{m,0}|^2 \right],$$

which implies that

$$\|f_{m+p}\| = 2^{(m-p)/2} \sqrt{|f_{m,-1}|^2 + |f_{m,0}|^2}. \quad (8.3.22)$$

Hence, $\|f - \Psi_{m+p}\| = \|f_{m+p}\| \leq C 2^{-p/2} \rightarrow 0$ as $p \rightarrow \infty$, where $C > 0$ is a constant. This not only completes the proof but also provides an algorithm (in fact a fast algorithm) for computation of the coefficients $c_{j,k}$ which are defined in (8.3.20). The function f is determined by 2^{m+n+1} individual function evaluations, and the coefficients $c_{j,k}$ require $2n$ evaluations, where this number increases with n .

This analysis implies that the expansion of a function $f \in L_2(R)$ is

$$f(t) = \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \langle f, \psi_{jk} \rangle \psi_{jk}(t), \quad (8.3.23)$$

which is convergent in the sense of $L_2(R)$. The standard approximation is given by the series

$$f_j(t) = \sum_{n=-\infty}^{j-1} \sum_{k=-\infty}^{\infty} \langle f, \psi_{nk} \rangle \psi_{nk}(t), \quad (8.3.24)$$

which converges to a piecewise constant function with jumps at $2^{-j}k$. Thus, $f_j \in V_j$, and since by Parseval's equality

$$\langle f_j, \phi_{jk} \rangle = \sum_{n=-\infty}^{j-1} \sum_{m=-\infty}^{\infty} \langle f, \psi_m \rangle \langle \psi_{jnm}, \phi_{jk} \rangle = \langle f, \phi_{jk} \rangle, \quad (8.3.25)$$

we find that f_j is a projection of f on V_j , i.e., $f = \sum_k \langle f, \phi_{jk} \rangle \phi_{jk}$. This gives a uniform pointwise convergence of $f_j \rightarrow f$. Note that the uniform convergence of f_j to f is not provided by the trigonometric system.

8.3.2. Wavelet Transform. In general, the wavelet transform of a time signal $f(t)$ is defined by

$$Wf(a, b) = \langle f, \psi_{ab} \rangle = \frac{1}{|a|^{1/2}} \int_{-\infty}^{\infty} f(t) \psi^*\left(\frac{t-b}{a}\right) dt, \quad (8.3.26)$$

where the double index a, b runs through the set $R^+ \times R$; the variable a is called the scaling parameter and b the translation parameter; the factor $1/|a|^{1/2}$ is for normalization so that $\|\psi_{ab}\| = 1$. For the wavelet transform there is an inversion formula which represents the original signal f as a 'linear combination' of the basis functions ψ_{ab} , where the values $Wf(a, b)$ of the wavelet transform become the coefficients. The characteristic volume element of the index set $R^+ \times R$ is defined by

$$f(t) = \frac{1}{C_\psi} \int_{R^+ \times R} Wf(a, b) \psi_{ab} \frac{da db}{|a|^2}. \quad (8.3.27)$$

The WFT of the Haar father wavelet $\phi(t)$ is given by

$$\Phi(\omega) = \frac{e^{-i\omega/2}}{\sqrt{2\pi}} \frac{\sin(\omega/2)}{\omega/2}, \quad (8.3.28)$$

and that of the mother wavelet $\psi(t)$ by

$$\Psi(\omega) = \frac{1}{\sqrt{2\pi}} \left\{ \int_0^{1/2} - \int_{1/2}^1 \right\} e^{-i\omega t} dt = \frac{i}{\sqrt{2\pi}} \frac{\sin^2(\omega/4)}{\omega/4} e^{-i\omega/2}. \quad (8.3.29)$$

The graph of $|\Psi(\omega)|$ is given in Fig. 8.3.5 (see page 543). The function $|\Psi(\omega)|$ has its first maximum at the frequency $\omega_0 \approx 4.6622$, and it decays like $1/\omega$ as $\omega \rightarrow \infty$, but very slowly at infinity because of the discontinuity of $\psi(t)$.

Consider a 'mother' wavelet $\psi(t)$ which is an infinitely differentiable, rapidly decaying function of t defined on R^n , with the Fourier transform $\Psi(\omega)$ which satisfies the following four conditions

- (i) $\Psi(\omega) = 1$ if $1 + \alpha \leq |\omega| \leq 2 - 2\alpha$, where $0 < \alpha \leq 1/3$,

- (ii) $\Psi(\omega) = 0$ if $|\omega| \leq 1 - \alpha$ or $|\omega| \geq 2 + 2\alpha$,
- (iii) $\Psi(\omega)$ is infinitely differentiable on R^n , and
- (iv) $\sum_{j=-\infty}^{\infty} |\Psi(2^{-j}\omega)|^2 = 1$ for all $\omega \neq 0$.

Note that the condition (iv) is satisfied by all orthonormal wavelet bases of the form $2^{j/2}\psi(2^jt - k)$.

If we set $\psi_j(t) = 2^{nj}\psi(2^kt)$ and replace the dyadic blocks (8.2.9) by the convolution products $\Delta_j f = f * \psi_j$, then the *Littlewood-Paley-Stein function* (see [Stein and Weiss 1971](#)) is defined by

$$g(t) = \sqrt{\sum_{j=-\infty}^{\infty} |\delta_j(f)(t)|^2}. \quad (8.3.30)$$

If $f \in L_2(R^n)$, so does g , and $\|f\|_2 = \|g\|_2$, which implies conservation of energy. Also, if $1 < p < \infty$, then for all $f \in L_p(R^n)$

$$c_p \|g\|_p \leq \|f\|_p \leq C_p \|g\|_p, \quad (8.3.31)$$

where $\|f\|_p = \left(\int_{R^n} |f(t)|^p dx \right)^{1/p}$. The inequalities (8.3.31) do not hold for $\alpha = 0$.

8.3.3. Ordered Fast Haar Wavelet Transform. The fast Haar wavelet transform is used to analyze a signal $f(t)$ in terms of the wavelets in the Haar family. This process begins by initialization of an array of $2^n = N$ entries and then goes through n iterations of the basis transform. For each index $m, m = 1, 2, \dots, n$, this array consists of 2^{n-m+1} coefficients of 2^{n-m+1} step functions $\phi_k^{(n-m+1)}$ defined by (8.3.4). After m iterations the array will contain 2^{n-m} coefficients (denoted by $a_k^{(n-m)}$) of the functions $\phi_k^{(n-m)}$ and 2^{n-m} coefficients (denoted by $b_k^{(n-m)}$) of the wavelets $\psi_k^{(n-m)}$ which are defined by (8.3.5). The step-by-step process is as follows.

INITIALIZATION. Given a sample (data) $\mathbf{s} = \{s_0, s_1, \dots, s_j, \dots, s_{2^n-1}\}$, we establish a one-to-one relation between \mathbf{s} and an array

$$\mathbf{a}^{(n)} = \{a_0^{(n)}, a_1^{(n)}, \dots, a_j^{(n)}, \dots, a_{2^n-1}^{(n)}\},$$

where the superscript (n) indicates that each array has 2^n elements ranging from 0 to $2^n - 1$. The array corresponds to the approximation \tilde{f} of a signal f , which is defined by

$$\tilde{f}(t) = \sum_{j=0}^{2^n-1} a_j^{(n)} \phi_j^{(n)}(t). \quad (8.3.32)$$

FIRST ITERATION. This iteration of the basic transform applied to all consecutive pairs $\{s_{2k}, s_{2k+1}\}$ of the initial array of the sample \mathbf{s} is such that $\mathbf{a}^{(n)} = \mathbf{s}$.

m -TH ITERATION. In the general case of the m -th iteration, the transform begins with the array

$$\mathbf{a}^{(n-m+1)} = \left\{ a_0^{(n-m+1)}, \dots, a_{2^{n-m+1}-1}^{(n-m+1)} \right\}, \quad (8.3.33)$$

which contains 2^{n-m+1} values. The basic transform is then applied to each pair $\left\{ a_{2k}^{(n-m+1)}, a_{2k+1}^{(n-m+1)} \right\}$, which yields two new 2^{n-m} pairs of coefficients

$$\begin{aligned} a_{2k}^{(n-m)} &= \frac{a_{2k}^{(n-m+1)} + a_{2k+1}^{(n-m+1)}}{2}, \\ b_{2k}^{(n-m)} &= \frac{a_{2k}^{(n-m+1)} - a_{2k+1}^{(n-m+1)}}{2}, \end{aligned} \quad (8.3.34)$$

which can be arranged into the following two arrays:

$$\begin{aligned} \mathbf{a}^{(n-m)} &= \left\{ a_0^{(n-m)}, a_1^{(n-m)}, \dots, a_j^{(n-m)}, \dots, a_{2^{n-m}-1}^{(n-m)} \right\}, \\ \mathbf{b}^{(n-m)} &= \left\{ b_0^{(n-m)}, b_1^{(n-m)}, \dots, b_j^{(n-m)}, \dots, b_{2^{n-m}-1}^{(n-m)} \right\}. \end{aligned} \quad (8.3.35)$$

Thus, at the m -th iteration we obtain the following arrays:

(i) The beginning array $\mathbf{a}^{(n-m+1)}$, defined by (8.3.33), which approximates the function f with 2^{n-m+1} steps of narrower width $2^{-(n-m+1)}$:

$$\tilde{f}^{(n-m+1)}(t) = \sum_{j=0}^{2^{n-m+1}-1} a_j^{(n-m+1)} \phi_j^{(n-m+1)}(t). \quad (8.3.36)$$

(ii) The final arrays $\mathbf{a}^{(n-m)}$ and $\mathbf{b}^{(n-m)}$, defined by (8.3.35), of which the former approximates f with 2^{n-m} steps of wider width 2^{m-n} :

$$\tilde{f}^{(n-m)}(t) = \sum_{j=0}^{2^{n-m}-1} a_j^{(n-m)} \phi_j^{(n-m)}(t), \quad (8.3.37)$$

and the latter approximates f with 2^{n-m} wavelets $\psi_j^{(n-m)}$ of wider width 2^{m-n} :

$$\hat{f}^{(n-m)}(t) = \sum_{j=0}^{2^{n-m+1}-1} b_j^{(n-m)} \psi_j^{(n-m)}(t). \quad (8.3.38)$$

Since the scaling function ϕ does not alter the sampled function but only represents it with different wavelets, the initial approximation $\tilde{f}^{(n-m+1)}(t)$ is the sum of (8.3.37) and (8.3.38), i.e.,

$$\tilde{f}^{(n-m+1)}(t) = \tilde{f}^{(n-m)}(t) + \hat{f}^{(n-m)}(t).$$

EXAMPLE 8.3.4. Consider the sample $\mathbf{s} = \{5, 1, 0, 6, 7, 3, 8, 4\}$, where $n = 3$.

INITIALIZATION. $\mathbf{a}^{(3)} = \mathbf{s} = \{5, 1, 0, 6, 7, 3, 8, 4\}$.

$$\begin{aligned}\text{FIRST ITERATION. } \mathbf{a}^{(2)} &= \left\{ \frac{5+1}{2}, \frac{0+6}{2}, \frac{7+3}{2}, \frac{8+4}{2} \right\} = \{3, 3, 5, 6\}, \\ \mathbf{b}^{(2)} &= \left\{ \frac{5-1}{2}, \frac{0-6}{2}, \frac{7-3}{2}, \frac{8-4}{2} \right\} = \{2, -3, 2, 2\},\end{aligned}$$

which is stored as

$$\mathbf{s}^{(2)} = \{\mathbf{a}^{(2)}; \mathbf{b}^{(2)}\} = \{3, 3, 5, 6; 2, -3, 2, 2\}.$$

$$\begin{aligned}\text{SECOND ITERATION. } \mathbf{a}^{(1)} &= \left\{ \frac{3+3}{2}, \frac{5+6}{2} \right\} = \left\{ 3, \frac{11}{2} \right\}, \\ \mathbf{b}^{(1)} &= \left\{ \frac{3-3}{2}, \frac{5-6}{2} \right\} = \left\{ 0, -\frac{1}{2} \right\},\end{aligned}$$

which is stored as

$$\mathbf{s}^{(1)} = \{\mathbf{a}^{(1)}; \mathbf{b}^{(2)}; \mathbf{b}^{(1)}\} = \left\{ 3, \frac{11}{2}; 0, -\frac{1}{2}; 2, -3, 2, 2 \right\}.$$

$$\begin{aligned}\text{THIRD ITERATION. } \mathbf{a}^{(0)} &= \left\{ \frac{3+11/2}{2} \right\} = \left\{ \frac{17}{4} \right\}, \\ \mathbf{b}^{(0)} &= \left\{ \frac{3-11/2}{2} \right\} = \left\{ -\frac{5}{4} \right\},\end{aligned}$$

which is stored as

$$\mathbf{s}^{(0)} = \{\mathbf{a}^{(0)}; \mathbf{b}^{(0)}; \mathbf{b}^{(1)}; \mathbf{b}^{(2)}\} = \left\{ \frac{17}{4}; -\frac{5}{4}; 0, -\frac{1}{2}; 2, -3, 2, 2 \right\}.$$

Thus, the approximation \tilde{f} , given by the initial data \mathbf{s} , is

$$\begin{aligned}\tilde{f}(t) &= 5\phi_{[0,1/8)}(t) + \psi_{[1/8,1/4)}(t) + 6\psi_{[3/8,1/2)}(t) + 7\psi_{[1/2,5/8)}(t) \\ &\quad + 3\psi_{[5/8,3/4)}(t) + 8\psi_{[3/4,7/8)}(t) + 4\psi_{[7/8,1)}(t),\end{aligned}$$

and by the final array $\mathbf{s}^{(0)}$ is

$$\begin{aligned}\tilde{f}(t) &= \frac{17}{4}\phi_{[0,1)}(t) - \frac{5}{4}\psi_{[0,1)}(t) + 0\psi_{[0,1/2)}(t) - \frac{1}{2}\psi_{[1/2,1)}(t) \\ &\quad + 2\psi_{[0,1/4)}(t) - 3\psi_{[1/4,1/2)}(t) + 2\psi_{[1/2,3/4)}(t) + 2\psi_{[3/4,1)}(t).\end{aligned}\tag{8.3.39}$$

Note that in the representation (8.3.39), the first term $\frac{17}{4}\phi_{[0,1)}(t)$ implies that the data \mathbf{s} has an average value of $\frac{17}{4}$; the second term $-\frac{5}{4}\psi_{[0,1)}(t)$ means that the data undergoes a jump in the opposite direction by $\frac{5}{4}$ times the size of the mother wavelet; the next two terms show an average jump of $-\frac{1}{2}$ in the first generation of daughter wavelets; and the last four terms show that the sample oscillates with jumps of 2, -3, 2, 2 in the second generation of the daughter wavelets. ■

8.4. Other Wavelet Systems

The Haar wavelet family is the simplest case of wavelets. There are many other wavelet families, where each family is generated by a scaling function (father wavelet) ϕ . Some important families are discussed below.

8.4.1. Schauder System. If the Haar functions $\psi(t)$ are replaced by their primitives, we obtain the Schauder basis as defined in Meyer (1993). Define

$$\Delta(t) = \begin{cases} 0 & t \notin [0, 1], \\ 2t & 0 \leq t \leq 1/2, \\ 2(1-t) & 1/2 \leq t \leq 1, \end{cases} \quad (8.4.1)$$

and consider the sequence $\{\Delta_n(t)\}$, $n \geq 1$, defined for $n = 2^j + k$ by

$$\Delta_n(t) = \Delta(2^j t - k) \quad j \geq 0, \quad 0 \leq k < 2^j. \quad (8.4.2)$$

The functions $\Delta_n(t)$ are defined on the interval $I_{j,k} = [k 2^j, (k+1) 2^{j-1}]$. Note that $\Delta_n(t)$ is the primitive of $\psi_{j,k}(t)$ multiplied by $2^{j/2+1}$, and has zeros outside $[0, 1]$. If we take $\Delta_0(t) = t$, then the sequence

$$\{1, \Delta_0(t), \Delta_1(t), \dots, \Delta_n(t)\}$$

is known as the *Schauder basis* of $f \in L_2$. Thus, every signal $f \in [0, 1]$ can be written as

$$f(t) = a + b t + \sum_{n=1}^{\infty} \alpha_n \Delta_n(t). \quad (8.4.3)$$

This series converges uniformly everywhere on $[0, 1]$, and therefore the coefficients α_n are uniquely determined as follows: Since $f(0) = a$, $f(1) = a + b$, which gives $b = f(1) - f(0)$. Then consider the function $f(t) = a - b t$, which has zeros at 0 and 1. This gives $\alpha_1 = f(1/2)$, $\alpha_2 = f_2(1/4)$, $\alpha_3 = f(3/4)$, and so on, and in general,

$$\alpha_n = f((k + 1/2) 2^j) - \frac{1}{2} [f(k 2^{-j}) + f((k + 1) 2^{-j})],$$

and $|\alpha_n| \leq C \cdot 2^{-(j+1)\eta}$, $0 < \eta < 1$.

The Haar system is not a Schauder basis of the Banach space \mathcal{X} since a Schauder basis of \mathcal{X} must contain vectors of \mathcal{X} , but the functions $\psi_{j,k}(t)$ are not continuous.

8.4.2. Shannon System. The Shannon scaling function is $\phi(t) = \frac{\sin(\pi t)}{\pi t}$, with its Fourier transform as

$$\Phi(\omega) = \chi_{[-\pi, \pi]}(\omega). \quad (8.4.4)$$

For the graph of $\phi(t)$ see Fig. 8.4.1 (see page 543). If the transform $F(\omega)$ is such that $\int_{-\infty}^{\infty} |F(\omega)|^2 d\omega < \infty$ for every ω , $|\omega| > \omega_0 > 0$, then from (8.4.4) we obtain the expansion formula, known as the Shannon sampling theorem:

$$f(t) = \sum_{n=-\infty}^{\infty} f(n) \frac{\sin \pi(t-x)}{\pi(t-x)}. \quad (8.4.5)$$

This theorem shows that if the signal f consists of only frequencies that do not exceed an upper limit ω_0 , then a sample of that signal at intervals of π/ω_0 is sufficient to reconstruct the signal. However, in practical applications we use only a finite number of sample points.

The Shannon sampling theorem also enables us to recover a band-limited function $f \in V_0$ from its values. On changing the scale in (8.4.5) by a factor of 2, we obtain a sampling theorem on the half-integers. The space with this new scale is V_1 and it contains a function whose Fourier transforms vanish outside the interval $[-2\pi, 2\pi]$. Continuing this process we increase the sequence of spaces. Instead of shrinking we can stretch the scale to obtain a sequence

$$\dots \subseteq V_{-m} \subseteq \dots \subseteq V \subseteq V_0 \subseteq V_1 \dots \subseteq V_m \subseteq \dots$$

Toward the left of this sequence the support of the Fourier transform shrinks to zero; toward the right it expands to all R . Thus,

- (i) $\bigcap_m V_m = \{0\}$;
- (ii) each $f \in L_2(R)$ can be approximated by a function in V_m for sufficiently large m .

The sequence $\{V_n\}$ is called a multiresolution analysis associated with $\phi(t)$. In the particular case when $f \in V_0$, which is composed of π band limited functions, we can write (8.4.5) as

$$f(t) = \sum_{n=-\infty}^{\infty} f(n) \phi(t-n).$$

A mother wavelet is given by

$$\psi(t) = \frac{\sin \pi(t-1/2) - \sin 2\pi(t-1/2)}{\pi(t-1/2)}, \quad (8.4.6)$$

the graph of which is given in Fig. 8.4.2 (see page 544). In the general case, a function ψ whose Fourier transform satisfies

$$\Psi(\omega) = e^{i\omega/2} \chi_I(\omega), \quad \text{where } I = [-2\pi, -\pi) \cup (\pi, 2\pi], \quad (8.4.7)$$

is called a Shannon wavelet. Since the Fourier transform of $\psi_{jk}(t)$ is

$$\mathcal{F}\{\psi_{jk}(t)\} = 2^{-j/2} \Psi(2^j \omega) e^{-2^{-j} k \omega}, \quad (8.4.8)$$

and since

$$\langle \psi_{jk}(t), \psi_{lm}(t) \rangle = \begin{cases} \frac{1}{2\pi} \langle \Psi_{jk}(\omega), \Psi_{lm}(\omega) \rangle = 0 & \text{for } j \neq l, \\ \delta_{km} & \text{for } j = l, \end{cases} \quad (8.4.9)$$

we conclude that ψ is an orthonormal wavelet for $L_2(R)$. To show that this system is also a basis, we use (8.1.3) and a change of variables to obtain

$$\begin{aligned} \sum_j \sum_k |\langle f, \psi_{jk} \rangle|^2 &= \sum_j \sum_k \frac{2^{-j}}{2\pi} \left| \int_R F(\omega) \Psi^*(2^{-j}\omega) e^{i2^{-j}k\omega} d\omega \right|^2 \\ &= \sum_j \frac{2^j}{\sqrt{2\pi}} \sum_k \left| \int_I F(2^j\omega) \frac{e^{ik\omega}}{\sqrt{2\pi}} d\omega \right|^2. \end{aligned} \quad (8.4.10)$$

Since $\left\{ \frac{e^{ik\omega}}{\sqrt{2\pi}} \right\}$ is an orthonormal basis of $L_2(R)$, which is equivalent to the orthogonality on $[0, 2\pi]$, we get from (8.4.10)

$$\begin{aligned} \sum_j \sum_k |\langle f, \psi_{jk} \rangle|^2 &= \sum_j \frac{2^j}{\sqrt{2\pi}} \left| \int_I F(2^j\omega) \right|^2 d\omega \\ &= \frac{1}{\sqrt{2\pi}} \sum_j \int_R \chi_I(2^{-j}\omega) |F(\omega)|^2 d\omega = \frac{1}{\sqrt{2\pi}} \|F(\omega)\|_2^2 = \|f(t)\|_2^2, \end{aligned} \quad (8.4.11)$$

where $\sum_j \chi_I(2^{-j}\omega) = 1$ for $\omega \in R$ a.e. Thus, $\psi(t)$ is an orthonormal wavelet for $L_2(R)$. Another Shannon wavelet is

$$\psi(t) = -2 \frac{\sin(2\pi t) + \cos(\pi t)}{\pi(2t+1)}. \quad (8.4.12)$$

A graph of this wavelet is given in [Fig. 8.4.3](#) (see page 544).

8.4.3. Franklin System. The Franklin system (Franklin 1928) defined below produces an orthonormal basis from the Schauder basis by using the Gram-Schmidt process, as follows. Start with a sequence $\{f_n(t)\}$ with $f_{-1}(t) = 1$, $f_0(t) = 2\sqrt{3}(t - 1/2), \dots$, such that $\int_0^1 f_n(t) dt = \int_0^1 t f_n(t) dt = 0$ for all $n \geq 1$. This sequence is an orthonormal basis for $L_2[0, 1]$ and is known as the Franklin system. It has advantages over the Haar and Schauder bases, but its drawback is that it has no simple algorithmic structure. Ciesielski (see [Meyer 1993](#)) proved that there exist constants $\gamma > 0$ and $C > 0$ such that

$$|f_n(t)| \leq C 2^{j/2} e^{-\gamma|2^j t - k|}, \quad t \in [0, 1], \quad n = 2^j + k, \quad 0 \leq k \leq 2^j, \quad (8.4.13)$$

$$\left| \frac{d}{dt} f_n(t) \right| \leq C 2^{3j/2} e^{-\gamma|2^j t - k|}. \quad (8.4.14)$$

Thus, $f_n(t) = 2^{j/2} \psi_S(2^j t - k)$, where $\psi_S(2^j t - k)$ is the Strömberg function which satisfies the Lipschitz condition on $[0, 1]$ (Strömberg 1981) and has the following properties: (a) $\psi_S(t) \in C(R^1)$; (b) $\psi_S(t)$ is linear on the intervals $[1, 2], [2, 3], \dots, [l, l+1], \dots$, and on $[\frac{1}{2}, 1], [0, \frac{1}{2}], [-\frac{1}{2}, 0], \dots, [-(l+1)/2, -l/2]$; (c) $|\psi_S(t)| \leq C(2 - \sqrt{3})^{|t|}$. This implies that $\psi_S(t)$ decays rapidly at infinity; and (d) $2^{j/2} \psi_S(2^j t - k)$ is an orthonormal basis for $L_2(R)$ since $2 - \sqrt{3} < 1$. Strömberg has given an asymptotic estimate for $f_n(t)$ as

$$f_n(t) = 2^{j/2} \psi_S(2^j t - k) + r_n(t) \quad \text{for } n = 2^j + k, \quad 0 \leq k \leq 2^j, \quad (8.4.15)$$

where $\|r_n(t)\|_2 \leq C(2 - \sqrt{3})^{d(n)}$, $d(n) = \inf\{k, 2^j - k\}$, and $C > 0$ is a constant.

8.4.4. Strömberg's System. Let $\mathcal{H}^1(R)$ denote the real Hardy space $H^1(R)$, which contains real-valued functions $u(t)$ such that $u(t) + i v(t) \in H^1(R)$. This means that $u \in \mathcal{H}^1(R)$ iff u and its Hilbert transform \hat{u} belong to $L_1(R)$. There are two approaches of 'atomic decomposition' (or wavelet analysis) of functions in $\mathcal{H}^1(R)$:

I. A function $f \in \mathcal{H}^1(R)$ can be written as (Coifman and Weiss 1977a)

$$f(t) = \sum_{k=0}^{\infty} \lambda_k A_k(t), \quad (8.4.16)$$

where λ_k are such that $\sum_{k=0}^{\infty} |\lambda_k| < \infty$, and $A_k(t)$ denote the 'atoms' of $\mathcal{H}^1(R)$; i.e., for each $A_k(t)$ there exists an interval I_k such that $|A_k(t)| \leq |I_k|^{-1}$ inside the interval I_k , and $A_k(t) = 0$ outside I_k , where $|I_k|$ denotes the length of the interval I_k , and $\int_{I_k} A_k(t) dt = 0$. These conditions imply that the norms of A_k in $\mathcal{H}^1(R)$ are bounded by a fixed constant C_0 .

II. Let $\{B_k(t)\}$ denote a sequence of functions in \mathcal{H}^1 , which are linearly independent, so that we can write

$$f(t) = \sum_{k=0}^{\infty} \beta_k B_k(t), \quad (8.4.17)$$

where the coefficients β_k are scalars, defined by $\beta_k = \int f(t) g_k(t) dt$, $g_k(t)$ being the functions in the dual of \mathcal{H}^1 . Thus, there exists a constant $C > 0$ such that if $|\beta_k| \leq |\lambda_k|$ for all k , then in the norm of the function space \mathcal{H}^1

$$\left\| \sum_{k=0}^{\infty} \beta_k B_k(t) \right\| \leq C \left\| \sum_{k=0}^{\infty} \lambda_k B_k(t) \right\|. \quad (8.4.18)$$

It is known that the Franklin system $f_0(t), f_1(t), \dots, f_n(t)$, without the function 1, is an unconditional basis for the subspace of $\mathcal{H}^1(R)$. Strömberg has proved that

the orthonormal basis defined by the function $\psi_S(t)$ is an unconditional basis for the subspace of $\mathcal{H}^1(R)$.

8.4.5. Lusin's System. Let $H^p(R)$, $1 \leq p < \infty$, denote the Hardy space, and let D denote the upper half-plane $\Im\{z\} = y > 0$. Then a function $f(z)$ belongs to $H^p(R)$ if it is regular in D and if

$$\sup_{y>0} \left(\int_{-\infty}^{\infty} |f(x + iy)|^p dx \right)^{1/p} < \infty. \quad (8.4.19)$$

and $f(z)$ converges to $f(x)$ as $y \rightarrow 0$, where convergence is in the sense of L_p -norm. Hardy spaces are very useful in the study of signal processing. Thus, given a real signal $f(t)$ of finite energy, $-\infty < t < \infty$, we can associate an analytic function $F(t)$ whose real part is $f(t)$. Since the energy of f is $\int_{-\infty}^{\infty} |f(t)|^2 dt < \infty$, we require that $F(t)$ should also have finite energy. This means that F belongs to the Hardy space $H^2(R)$. Then $F(t) = f(t) + i g(t)$ is the Hilbert transform of $f(t)$; for analytic signals, see [Papoulis \(1988\)](#).

The analysis of functions in $H^p(R)$ is carried out by using ‘atoms’ (or basis elements) which are elementary functions in $H^p(R)$. One such function is $(z - w^*)^{-2}$, where w^* denotes the complex conjugate of $w \in D$. Then a function $f \in H^p(R)$ is represented by

$$f(z) = \int_D (z - w^*)^{-2} \alpha(w) du dv, \quad w = u + iv, \quad (8.4.20)$$

where $\alpha(w)$ denotes the coefficients which are simple to calculate.

The synthesis of functions in $H^p(R)$ is obtained by the following rule: Start with an arbitrary measurable function $\alpha(w)$ subject to the Lusin's condition which states that the quadratic functional $A(x)$, known as Lusin's area function, must be such that

$$\int_{-\infty}^{\infty} [A(x)]^p dx < \infty, \quad \text{and} \quad A(x) = \sqrt{\iint_{\Gamma(x)} |\alpha(u + iv)|^2 v^{-2} du dv}, \quad (8.4.21)$$

where $\Gamma(x) = \{(u, v) \in R^2 : v > |u - x|\}$. Then

$$f(z) = \iint_D (z - w^*)^{-2} \alpha(w) du dv \in H^p(R),$$

and

$$\|f\|_p < C(p) \left(\int_{-\infty}^{\infty} [A(x)]^p dx \right)^{1/p}, \quad 1 \leq p < \infty,$$

where $\|f\|_p$ is the norm of f defined by (8.4.19). But this estimate is sometimes very crude; for example, for $f(z) = (z + i)^{-2}$ the value of $\iint_D (z - w^*)^{-2} \alpha(w) du dv$

is not unique if we choose the Dirac measure at the point i for $\alpha(w)$. For a unique decomposition we choose $\alpha(w)$ only as $\alpha(w) = \frac{2i}{\pi} v f'(u + i v)$. Then the two norms $\|f\|_p$ and $\|A\|_p$ are the same for $1 \leq p < \infty$.

8.4.6. Grossmann and Mortel's System. Grossmann and Mortel (1984) define wavelets generated from the above analyzing wavelets $\psi(t)$ as

$$\psi_{a,b}(t) = a^{-n/2} \psi\left(\frac{t-b}{a}\right), \quad a > 0, b \in R^n. \quad (8.4.22)$$

These wavelets make an orthonormal basis and are very useful in the analysis and synthesis of an arbitrary function $f \in L_2(R^n)$. The wavelet coefficients are defined by

$$W(a, b) = \langle f, \psi_{a,b} \rangle. \quad (8.4.23)$$

The *analysis* of the function f is carried out by (8.4.23); its *synthesis* is given by

$$f(t) = \int_0^\infty \int_{R^n} W(a, b) \psi_{a,b} db \frac{da}{a^{n+1}}. \quad (8.4.24)$$

EXAMPLE 8.4.1. In the Hardy space $H^p(R)$, $1 \leq p < \infty$, the analyzing wavelet is $\psi(t) = \frac{1}{(t+i)^2}$, which is regular in D . Its Fourier transform is $\Psi(\omega) = \begin{cases} -2\omega e^{-\omega\pi} & \text{for } \omega \geq 0, \\ 0 & \text{for } \omega \leq 0. \end{cases}$ The condition (w.24) yields

$$\int_0^\infty |\Psi(t\omega)|^2 \frac{dt}{t} = \int_0^\infty |-2t\omega e^{-t\omega}|^2 \frac{dt}{t} = \begin{cases} 1 & \text{if } \omega > 0, \\ 0 & \text{if } \omega \leq 0. \end{cases}$$

Thus, the Calderón's condition is not satisfied. The wavelets $\psi_{a,b}(t)$ generate $H^2(R)$ instead of $L_2(R)$ when $a > 0$ and $b \in R$, and the wavelet coefficients of the function $f \in H^2(R)$ are

$$W(a, b) = \langle f, \psi_{a,b} \rangle = \frac{1}{\pi} \int_{-\infty}^\infty f(t) \frac{a\sqrt{a}}{(t-b-ia)^2} dt = 2i a\sqrt{a} f'(b+ia),$$

since f is regular in D . ■

EXAMPLE 8.4.2. Consider $\psi(t) = 1/(t+i)$, which belongs to all Hardy spaces. Since its Fourier transform is $\Psi(\omega) = i\sqrt{2\pi} e^{-\omega}$, we find that $\int_0^\infty |\Psi(t\omega)|^2 \frac{dt}{t} = +\infty$ if $\omega > 0$. Hence, this $\psi(t)$ cannot be used as an analyzing wavelet. ■

8.4.7. Hat Wavelet System. The hat wavelet scaling function is defined by (see Aboufadel and Schlicker 1999)

$$\phi(t) = \begin{cases} t, & 0 \leq t < 1, \\ 2-t, & 1 \leq t < 2, \\ 0, & \text{elsewhere,} \end{cases} \quad (8.4.25)$$

For a graph of this function see Fig. 8.4.4 (see page 544). This scaling function is not orthogonal to all of its translates. There exist integers k such that $\langle \phi(t), \phi(t-k) \rangle \neq 0$.

8.4.8. Quadratic Battle-Lemarié System. The scaling function is defined by (see Aboufadel and Schlicker 1999)

$$\phi(t) = \begin{cases} \frac{1}{2} t^2, & 0 \leq t < 1, \\ -t^2 + 3t - \frac{3}{2}, & 2 \leq t < 3, \\ \frac{1}{2} (t-3)^2, & 1 \leq t < 2, \\ 0, & \text{elsewhere,} \end{cases} \quad (8.4.26)$$

For a graph of this function see Fig. 8.4.5 (see page 545). Like the hat wavelet, this scaling function is also not orthogonal to all of its translates.

8.4.9. Mexican Hat Wavelet System. The Mexican hat (or Maar) function $\psi(t)$ is defined by the second derivative of the Gaussian $e^{-t^2/2}$ with the normalization such that its L_2 -norm is $\|\psi(t)\|_2 = 1$, i.e.,

$$\psi(t) = \frac{2}{\sqrt{3}} \pi^{-1/4} (1 - t^2) e^{-t^2/2}. \quad (8.4.27)$$

Its Fourier transform is

$$\Psi(\omega) = \frac{2}{\sqrt{3}} \pi^{-1/4} \omega^2 e^{\omega^2/2}. \quad (8.4.28)$$

The Mexican hat function $\psi(t)$ is such that $\int_{-\infty}^{\infty} \psi(t) dt = 0$, and

$$C_\psi = 2\pi \int_{-\infty}^{\infty} |\Psi(\omega)|^2 |\omega|^{-1} d\omega = \frac{8}{3} \pi^{-1/4} < \infty. \quad (8.4.29)$$

For a graph of this function see Fig. 8.4.6 (see page 545). This wavelet is discussed in Foufoula-Georgion and Kumar (1994). This family has no simple scaling function, and in this respect it is different from other wavelet systems.

8.4.10. Meyer System. The Meyer wavelets are

$$\psi^{a,x}(t) = |a|^{-1/2} \psi\left(\frac{t-x}{a}\right) \quad \text{for } a, x \in \mathbb{R}, a \neq 0. \quad (8.4.30)$$

Then $\langle f, \psi^{a,x} \rangle \leq \|f\|$. For any $f, g \in L_2(\mathbb{R})$ we have

$$\begin{aligned} & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle f, \psi^{a,x} \rangle \langle g, \psi^{a,x} \rangle^* \frac{da db}{a^2} \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} F(\omega) |a|^{1/2} e^{-ix\omega} [\Psi(a\omega)]^* d\omega \right] \\ & \quad \times \left[\int_{-\infty}^{\infty} [G(\omega)]^* |a|^{1/2} e^{ix\omega'} [\Psi(a\omega')] d\omega' \right] \frac{da db}{a^2} \\ &= 2\pi \int_{-\infty}^{\infty} \frac{da}{|a|} \int_{-\infty}^{\infty} F(\omega) [G(\omega)]^* |\Psi(a\omega)|^2 d\omega \\ &= \frac{8}{3} \sqrt{\pi} < \langle f, g \rangle, \end{aligned}$$

which yields

$$\int_{-\infty}^{\infty} \int_0^{\infty} \langle f, \psi^{a,x} \rangle \langle g, \psi^{a,x} \rangle^* \frac{da db}{a^2} = \frac{4}{3} \sqrt{\pi} < \langle f, g \rangle. \quad (8.4.31)$$

8.4.11. Wavelet Analysis and Synthesis. For wavelet analysis, we consider the L_p space. Some observations are noted here.

(a) For the space $L_p[0, 2\pi]$, $1 \leq p < \infty$, the functions $\cos kt$ and $\sin kt$ cannot be the ‘atoms’, because these functions do not provide simple and useful assembly rules.

(b) The simplest atomic decomposition (or wavelet analysis) for the spaces $L_p[0, 1]$, $1 \leq p < \infty$, is provided by the Haar system. The Franklin system also gives a simple atomic decomposition.

(c) From the point of view of wavelet theory the Franklin system and the Littlewood-Paley analysis are related.

(d) For a simple approach to ‘atomic decomposition’ we can use Calderón’s identity which is as follows: Let $\psi(x) \in L_2(R^n)$ be the so-called analyzing wavelet (by Grossman and Morlet, see §8.1.8). Its Fourier transform $\Psi(\omega)$ is subject to the condition

$$\int_0^{\infty} |\Psi(t\omega)|^2 \frac{dt}{t} = 1 \quad \text{for almost all } \omega \in R^n. \quad (8.4.32)$$

If $\psi \in L_1(R^n)$, this condition becomes

$$\int_{R^n} \psi(x) dx = 0. \quad (8.4.33)$$

Write $\psi^*(x) = (\psi(-x))^*$, $\psi_t(x) = t^{-n}\psi(x/t)$, and $\Psi_t(x) = t^{-n}\Psi(x/t)$. Let Q_t denote the operator defined as convolution with ψ_t , and let its adjoint operator be denoted by Q_t^* . The *Calderón’s identity* is a decomposition of the identity operator defined by

$$I = \int_0^{\infty} Q_t Q_t^* \frac{dt}{t}. \quad (8.4.34)$$

The first synthesis is to relate the Littlewood-Paley decomposition (1930), Franklin system revised by Strömberg, and the Calderón’s identity. This synthesis is based on the definition of the words ‘wavelet’ and the related wavelet transform. There are three basic definitions:

FIRST DEFINITION. (Grossmann-Morlet, §8.4.8) A wavelet is a function $\psi \in L_2(R)$ whose Fourier transform $\Psi(\omega)$ satisfies the condition (8.4.32).

SECOND DEFINITION. (Littlewood-Paley-Stein, §8.3.2) A wavelet is a function $\psi \in L_2(R^n)$ whose Fourier transform $\Psi(\omega)$ is such that $\sum_{j=-\infty}^{\infty} |\Psi(2^{-j}\omega)|^2 = 1$ almost everywhere.

THIRD DEFINITION. (Franklin-Strömberg, §8.4.3 and §8.4.4) A wavelet is a function $\psi \in L_2(R)$ such that $2^{j/2}\psi(2^j t - k)$ is an orthonormal basis for $L_2(R)$.

In going from the first to the third definition we have increased the number of conditions, thereby narrowing the scope of wavelets. The wavelet analysis of functions does the same thing: In Grossmann-Morlet's definition the wavelet analysis of a function ψ yields a function $W(a, b)$ of $n + 1$ variables $a > 0$ and $b \in R^n$, where the function $W(a, b)$ is defined by (4.8.23). In Littlewood-Paley, a is replaced by 2^{-j} , and b is denoted by t . Thus, if G denotes the multiplicative group $\{2^{-j}\}$, then Littlewood-Paley analysis is obtained by carrying out the Grossmann-Morlet's analysis on $G \times R^n$. In Franklin-Strömberg analysis a is replaced by 2^{-j} and b by ka^{-j} .

In these three cases the wavelet synthesis deals with the reconstruction of $f(t)$ from its wavelet transform. In Grossmann-Morlet wavelets this synthesis is given by (4.8.24). In Littlewood-Paley case the integral $\int_0^\infty u(a) \frac{da}{a}$ is replaced by the sum $\sum_{j=-\infty}^{\infty} u(2^{-j})$, and the synthesis (4.8.24) becomes

$$f(t) = \sum_{j=-\infty}^{\infty} \int_{R^n} (\Delta_j^* f)(b) \psi_j(t - b) db. \quad (8.4.35)$$

For the Strömberg's orthogonal wavelets the integral in (8.4.35) reduces to a sum in the case $n = 1$ and the synthesis is then given by

$$f(t) = \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \alpha(j, k) \psi_{j,k}(t). \quad (8.4.36)$$

8.5. Daubechies' System

The orthonormal bases of the form $2^{j/2}\psi(2^j t - k)$, where $\psi \in C^1$ with compact support, were discovered by Daubechies (1988). For each integer r there exists an orthonormal basis of $L_2(R)$ of the form $2^{j/2}\psi_r(2^j t - k)$, such that (i) the support of ψ_r is the interval $[0, 2r + 1]$; (ii) $0 = \int_{-\infty}^{\infty} \psi_r(r) dt = \dots = \int_{-\infty}^{\infty} t^r \psi_r(r) dt$; and (iii) $\psi_r(t)$ has γr continuous derivatives, where $\gamma \approx 1/5$. For $r = 0$ this system reduces to the Haar system.

The Daubechies wavelets are more effective in both analysis and synthesis than the Haar system. For example, if the function f being analyzed has m continuous derivatives, $0 \leq m \leq r + 1$, then the coefficients $\alpha(j, k)$ from its decomposition in the Daubechies basis are of the order of magnitudes $2^{-(m+1/2)j}$, whereas it is of order $2^{-3j/2}$ in the Haar system ($m = 1$). It means that while computing $f(t)$, the coefficients that are retained (i.e., those exceeding the machine precision) are much less than those in the Haar system. This process is known as 'signal compression'. Similarly the synthesis obtained by using the Daubechies system is far better than the Haar system. This system is composed of a wavelet family that has compact support and some smoothness. We will discuss the one-dimensional case. The Daubechies wavelets satisfy the following requirements: (a) The scaling function $\phi(t)$ has compact support (or finite duration of time) and $\phi(t) = 0$ outside the interval $[0, 3]$. Thus, all refinement coefficients are zeros except c_0, c_1, c_2 and c_3 , which implies that

$$\phi(t) = c_0 \phi(2t) + c_1 \phi(2t - 1) + c_2 \phi(2t - 2) + c_3 \phi(2t - 3). \quad (8.5.1)$$

(b) The class of wavelets so constructed is satisfied by the orthogonality condition, which requires that the scaling function $\phi(t)$ be orthogonal to its translates $\{\phi(t - k)\}$. Since by Parseval's formula $\sum_{k=-\infty}^{\infty} c_k = 2$ and $\sum_{k=-\infty}^{\infty} c_k c_{k-2j} = 0$ for every integer $j \neq 0$, this class of wavelets satisfies the conditions

$$\begin{aligned} c_0^2 + c_1^2 + c_2^2 + c_3^2 &= 2, \\ c_0 c_2 + c_1 c_3 &= 0, \\ c_0 c_3 - c_1 c_2 + c_2 c_1 - c_3 c_0 &= 0. \end{aligned} \quad (8.5.2)$$

This condition, known as the *regularity condition*, demands the smoothness of the scaling function $\phi(t)$ so that a smoother scaling function produces a better approximation for polynomials $p(t)$ and functions (or signals) $f(t)$. Thus, we must be able to express all constants, linear polynomials and signals as a linear combination of the elements $\{\phi(t - k)\}$.

The Daubechies scaling function $\phi(t)$ is constructed recursively by assuming the initial values

$$\phi(0) = 0, \quad \phi(1) = \frac{1 + \sqrt{3}}{2}, \quad \phi(2) = \frac{1 - \sqrt{3}}{2}, \quad \phi(3) = 0, \quad (8.5.3)$$

such that the function $\phi(t)$ satisfies the recurrence relation (8.5.1), where

$$c_0 = \frac{1 + \sqrt{3}}{4}, \quad c_1 = \frac{3 + \sqrt{3}}{4}, \quad c_2 = \frac{3 - \sqrt{3}}{4}, \quad c_3 = \frac{1 - \sqrt{3}}{4}, \quad (8.5.4)$$

are known as the *Daubechies coefficients*. Note that $\phi(0) + \phi(1) + \phi(2) + \phi(3) = 1$.

EXAMPLE 8.5.1. Using (8.5.1)–(8.5.3) we get

$$\begin{aligned}\phi(1/2) &= c_0 \phi(1) + c_1 \phi(0) + c_2 \phi(-1) + c_3 \phi(-2) \\ &= \frac{1 + \sqrt{3}}{4} \frac{1 + \sqrt{3}}{2} = \frac{2 + \sqrt{3}}{4}; \\ \phi(3/2) &= c_0 \phi(3) + c_1 \phi(2) + c_2 \phi(1) + c_3 \phi(0) \\ &= \frac{3 + \sqrt{3}}{4} \frac{1 - \sqrt{3}}{2} + \frac{3 - \sqrt{3}}{4} \frac{1 + \sqrt{3}}{2} = 0; \\ \phi(5/2) &= c_0 \phi(5) + c_1 \phi(4) + c_2 \phi(3) + c_3 \phi(2) \\ &= \frac{1 + \sqrt{3}}{2} \frac{1 - \sqrt{3}}{2} = \frac{2 - \sqrt{3}}{4}.\end{aligned}$$

For values of t which are odd multiples of $1/4$, we use the recursion (8.5.1) and obtain the following values:

t	1/4	3/4	5/4	7/4	9/4	11/4
$\phi(t)$	$\frac{5+3\sqrt{3}}{16}$	$\frac{9+5\sqrt{3}}{16}$	$\frac{1+\sqrt{3}}{8}$	$\frac{1-\sqrt{3}}{8}$	$\frac{9-5\sqrt{3}}{16}$	$\frac{5-3\sqrt{3}}{16}$ ■

The associated Daubechies ‘mother’ wavelet $\psi(t)$ is defined by the recurrence relation

$$\psi(t) = -c_0 \phi(2t) + c_1 \phi(2t - 1) - c_2 \phi(2t - 2) + c_3 \phi(2t - 3). \tag{8.5.5}$$

Note that $\psi(t) = 0$ if $2t + 2 \geq 0$ or $3 \leq 2t - 1$, i.e., if $t \leq -1$ or $2 \leq t$. Thus, the recursion (8.5.5) yields the Daubechies wavelet $\psi(t)$ for $-1 < t < 2$. For example, using (8.5.4)–(8.5.5) we obtain the following values:

t	-1	-1/2	0	1/2	1	3/2	2
$\psi(t)$	0	-1/4	$\frac{1-\sqrt{3}}{2}$	$\sqrt{3}$	$-\frac{1-\sqrt{3}}{2}$	-1/4	0

The above recursion produces the values of $\phi(t)$ and $\psi(t)$ only at integral multiples of positive or negative powers of 2. These values are sufficient for equally-spaced samples from a signal $f(t)$ since the signal remains unknown between the sample values. We will use the values that are known as dyadic, which makes a number field containing numbers of the form $p + q \sqrt{3}$ and follows the same rule for addition and multiplication as the complex numbers.

The graph for the Daubechies wavelet $\psi(t)$ can be obtained by using the Matlab command: > wave=MakeWavelet(2,-4,‘Daubechies’, 4, ‘Mother’ 3072).

The Daubechies wavelets satisfy the following conditions:

$$\text{Recursion:} \quad \phi(t) = \sum_{k=0}^N c_k \phi(2t - k), \quad N = 2^n, \quad (8.5.6)$$

$$\text{Wavelet:} \quad \psi(t) = \sum_{k=1-N}^1 (-1)^k c_{1-k} \phi(2t - k), \quad (8.5.7)$$

$$\text{Existence:} \quad \sum_{k=0}^{[N/2]} c_k = 1 = \sum_{k=0}^{[(N-1)/2]} c_{2k+1}, \quad (8.5.8)$$

$$\text{Orthogonality:} \quad \int_R \phi(2t - k) \phi(2t - m) = 0 \quad \text{for } k \neq m, \quad (8.5.9)$$

$$\sum_{k=\max\{0, 2m\}}^{\min\{N, N+2m\}} c_k c_{k-2m} = \begin{cases} 2 & \text{if } m = 0, \\ 0 & \text{if } m \neq 0. \end{cases} \quad (8.5.10)$$

The recursion (8.5.6) can be written for each $j = 1, \dots, N-1$ as

$$\phi(j) = \sum_{k=0}^N c_k \phi(2j - k),$$

which when listed for each j yields a linear system of $N-1$ equations

$$\phi(1) = c_1 \phi(1) + c_0 \phi(2),$$

$$\phi(2) = c_3 \phi(1) + c_2 \phi(2) + c_1 \phi(3) + c_0 \phi(4),$$

$$\vdots$$

$$\phi(N-2) = c_N \phi(N-4) + c_{N-1} \phi(N-3) + c_{N-2} \phi(N-2) + c_{N-3} \phi(N-1),$$

$$\phi(N-1) = c_{N-1} \phi(N-2) + c_{N-1} \phi(N-1).$$

This system can be written in matrix form as $\phi = \mathbf{H}\phi$, where

$$\phi = [\phi(1) \quad \phi(2) \quad \dots \quad \phi(N-2) \quad \phi(N-1)]^T,$$

$$\mathbf{H} = \begin{bmatrix} c_1 & c_0 & & & & \\ c_3 & c_2 & c_1 & c_0 & & \\ c_5 & c_4 & c_3 & c_2 & c_1 & c_0 \\ \vdots & & & & \ddots & \\ & & & & & c_N & c_{N-1} & c_{N-2} & c_{N-3} \\ & & & & & & c_N & c_{N-1} \end{bmatrix},$$

where the element h_{ij} of the matrix \mathbf{H} are given by

$$h_{ij} = \begin{cases} c_{2i-j} & \text{if } 2i-j = 0, \dots, N, \\ 0 & \text{if } 2i-j \neq 0, \dots, N. \end{cases}$$

Thus, the odd columns of \mathbf{H} contain the coefficients with odd indices and the even columns those with even indices. Also, in view of the condition (8.5.8), we have $\sum_{k=0}^{[n/2]} c_{2k} = 1 = \sum_{k=0}^{[(N-1)/2]} c_{2k+1}$, which means that each column of the matrix \mathbf{H} adds up to unity. Hence, the vector $\mathbf{1} = [1 \ 1 \ \dots \ 1 \ 1]^T$ is the eigenvector with eigenvalue 1 for the transposed matrix \mathbf{H}^T , and $\mathbf{H}^T \mathbf{1} = \mathbf{1}$. Since \mathbf{H}^T and \mathbf{H} have the same eigenvalue, \mathbf{H} will also have the eigenvalue 1 for some eigenvector ϕ . Thus, $\phi(j) = t_j$ is the value of ϕ at an integer j , and by (8.5.6) we can find the values of ϕ at all dyadic points as of the form $\phi(k/2^m)$ for each positive integer m and all integers $k = 0, \dots, 2^m N$.

EXAMPLE 8.5.2. For $N = 3$ (i.e., $n = 2$) consider the coefficients c_0, c_1, c_2, c_3 defined by (8.5.4). Here, $c_0 + c_2 = 1 = c_1 + c_3$; also, the matrix \mathbf{H} is given by

$$\mathbf{H} = \begin{bmatrix} c_1 & c_0 \\ c_3 & c_1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 3 + \sqrt{3} & 1 + \sqrt{3} \\ 1 - \sqrt{3} & 3 - \sqrt{3} \end{bmatrix},$$

and has eigenvalues 1 and $\frac{1}{2}$. We may note in passing that the matrix \mathbf{H} has the eigenvectors $[-1 \ 1]^T$ and $\left[-\frac{1 + \sqrt{3}}{1 - \sqrt{3}} \ 1\right]^T$. Since $\phi(0) = 0 = \phi(3)$, we solve the system $(\mathbf{H} - \mathbf{I})\phi = \mathbf{0}$, where $\phi = [\phi(1) \ \phi(2)]^T$, and find $\phi(1)$ and $\phi(2)$ to be the same as defined by (8.5.3), so that $\phi(1) + \phi(2) = 1$ approximates $\int_R \phi dt = 1$ by using the repeated midpoint quadrature rule. In fact, for all types of wavelet system that satisfy the conditions (8.5.6)–(8.5.10) the sum of the values of ϕ at all integers is always equal to unity and the integral of ϕ is also equal to unity, i.e.,

$$\sum_j \phi(j) = 1 \quad \text{and} \quad \int_R \phi dt = 1. \quad (8.5.11)$$

These results can be proved as follows:

$$\begin{aligned} \sum_j \phi(j/2^{m+1}) 2^{-(m+1)} &= \sum_j \sum_{k=0}^N c_k \phi(2(j/2^{m+1}) - k) 2^{-(m+1)} \\ &= \sum_j \sum_{k=0}^N c_k \phi(j/2^m - k) 2^{-(m+1)} \\ &= \sum_j \sum_{k=0}^N c_k \phi\left(\frac{j - 2^m k}{2^m}\right) 2^{-(m+1)} \\ &= \sum_{k=0}^N c_k \sum_j \phi\left(\frac{j - 2^m k}{2^m}\right) 2^{-(m+1)} \\ &= \frac{1}{2} \sum_{k=0}^N c_k \sum_j \phi(j/2^m) 2^{-m} = \frac{1}{2} \sum_{k=0}^N c_k = 1; \end{aligned}$$

$$\int_R \phi(t) dt = \int_0^N \phi(n) dn = \lim_{m \rightarrow \infty} \sum_j \phi(j/2^m) 2^{-m} = \lim_{m \rightarrow \infty} 1 = 1.$$

8.5.1. Approximation of Functions. The Daubechies scaling function $\phi(t)$ and the ‘mother’ wavelet $\psi(t)$ can both be used to approximate a function f which represents a signal, but unlike the Haar wavelet which interpolates signals at the sample points (data) in discontinuous steps, the Daubechies system yields a smoother approximation \tilde{f} of f which is known only from the set of sample points

$$\mathbf{s} = \{s_0, s_1, \dots, s_{2^n-2}, s_{2^n-1}\}. \quad (8.5.12)$$

For the sake of simplicity we assume that the sample points of a signal f are at integer point so that $s_k = f(k)$. These points are equally spaced if we use the transformation $g(k) = f(k/m)$ so that $s_k = g_k = f(k/m)$. Thus, the Daubechies wavelets start the approximation with the sample \mathbf{s} and use multiples of shifted basic scaling function ϕ , thus giving

$$\tilde{f}(t) = \sum_{k=-2}^{2^n-1} a_k \phi(t-k). \quad (8.5.13)$$

Note that the translations $\phi(t-k)$ of $\phi(t)$ by integers $k < 2$ or $k > 2^n - 1$ are zero for $0 \leq t \leq 2^n$.

EXAMPLE 8.5.3. We choose a set of equally spaced sample points $\{1/2, 3/2, 5/2,$ and find that $\phi(1/2) = 0.9330127$, $\phi(3/2) = 0$ and $\phi(5/2) = 0.0669872$. This approximates $f(0)\phi(1/2) \approx f(0)$, $f(1)\phi(3/2) = 0$, and $f(2)\phi(5/2) \approx 0$. Thus, $\tilde{f}(t) = f(0)$, which almost approximates the signal $f(t)$ at the point $1/2$, and the relative error (which is relative to the values of f with maximum magnitude) in this approximation is $|1 - 0.9330127| + |0 - 0| + |0 - 0.0669872| \approx 1.34 \times 10^{-2}$. Let us consider three equally spaced points $t_0 = \frac{3 - \sqrt{3}}{2}$, $t_1 = \frac{5 - \sqrt{3}}{2}$, and $t_2 = \frac{7 - \sqrt{3}}{2}$. Then since

$$\frac{649}{1024} < t_0 < \frac{650}{1024}, \quad \frac{1673}{1024} < t_1 < \frac{1674}{1024}, \quad \frac{2697}{1024} < t_2 < \frac{2698}{1024},$$

we obtain three sets of equally spaced points

$$\left\{ \frac{649}{1024}, \frac{1673}{1024}, \frac{2697}{1024} \right\}, \quad \{t_0, t_1, t_2\}, \quad \left\{ \frac{650}{1024}, \frac{1674}{1024}, \frac{2698}{1024} \right\}.$$

If we choose the last set, then $\phi(t_0) = 0.999985$, $\phi(t_1) = -0.000155$ and $\phi(t_2) = 0.00017$. Thus, $f(0)\phi(t_0) \approx f(0)$, $f(1)\phi(t_1) \approx 0$, and $f(2)\phi(t_2) \approx 0$. Thus, $\tilde{f}(t) = f(0)$, and the relative error in this approximation is $|1 - 0.999985| + |0 + 0.000155| + |0 - 0.00017| \approx 3.4 \times 10^{-4}$. For the first set we obtain a similar result, but since $\phi(t_0) = 1 = \phi(t_1) = \phi(t_2)$, the set $\{t_0, t_1, t_2\}$ yields the same result as that obtained by the set $\{1/2, 3/2, 5/2\}$. ■

The simplest case of choosing the coefficients a_k in (8.5.13) is to take $a_k \equiv s_k$ for each $k = 0, 1, \dots, 2^n - 1$. This leads to the approximation

$$\tilde{f}(t) = \sum_{k=0}^{2^n-1} s_k \phi(t-k), \quad (8.5.14)$$

which is an interpolation of f at the sample points (data) $s_k = f(k)$. For the sake of simplicity we will consider examples in the sequel with $n = 2$. For values of $n > 2$ the procedures can be extended similarly. Thus, for $n = 2$ the coefficient a_0 can be expressed as an average of the data $\mathbf{s} = \{s_0, s_1, s_2, s_3\}$ weighted by the corresponding values of ϕ , which gives

$$a_0 = s_0 \phi(0) + s_1 \phi(1) + s_2 \phi(2) + s_3 \phi(3). \quad (8.5.15)$$

In the sequel we will present examples with this data set \mathbf{s} .

EXAMPLE 8.5.4. Let the sample be $\mathbf{s} = \{s_0, s_1, s_2, s_3\} = \{0, 1, 2, 3\}$. Then, from (8.5.15) and (8.5.1) we find that $a_0 = \frac{3-\sqrt{3}}{2} \approx 0.633974596$, and the approximation \tilde{f} with this data contains $a_0 \phi$. ■

There are some different methods for computing the initial coefficients a_k near the edges (start and end) of a given sample, which help alleviate the edge effects in computing the approximation $\tilde{f}(t)$ of a signal $f(t)$. We will discuss the following three methods in detail (see Blatter 1998, Nievergelt 1999).

METHOD 1. The distorted edge effects are alleviated by extending zeros before and after the sample \mathbf{s} . The example given below explains how this method works in producing distorted approximations near the edges of a sample. Let $\mathbf{s} = \{s_0, s_1, s_2, s_3\} = \{f(0), f(1), f(2), f(3)\}$ be extended at both edges so that the extended sample becomes

$$\{s_{-4}, s_{-3}, s_{-2}, s_{-1}; s_0, s_1, s_2, s_3; s_4, s_5, s_6, s_7\}.$$

Then each coefficient a_k is computed by a weighted average technique, called a *convolution* of the extended sample weighted by the shifted scaling function, i.e., for each (negative, zero and positive) integer k

$$a_k = \sum_{t=n}^{n+3} s_t \phi(t-k). \quad (8.5.16)$$

EXAMPLE 8.5.5. (Nievergelt 1999) Consider a sample $\mathbf{s} = \{s_0, s_1, s_2, s_3\} = \{0, 1, 2, 3\}$, and let the extended sample be

$$\begin{array}{cccccccccccccccc} \{ & s_{-4} & s_{-3} & s_{-2} & s_{-1}; & s_0 & s_1 & s_2 & s_3; & s_4 & s_5 & s_6 & s_7 & \} \\ = \{ & 0 & 0 & 0 & 0 & ; & 0 & 1 & 2 & 3 & ; & 0 & 0 & 0 & 0 & \} \end{array}$$

The coefficient a_0 has been computed in Example 8.5.4. For $k \neq 0$, we align the values of t , $\phi(t-k)$ and s_t in the following tabular form which helps a visual setup. Thus, to compute a_1 the sample \mathbf{s} is weighted by $\phi(t-1)$, and we get

t	-4	-3	-2	-1	0	1	2	3	4	5	6	7
$\phi(t-1)$	0	0	0	0	0	0	$\frac{1+\sqrt{3}}{2}$	$\frac{1-\sqrt{3}}{2}$	0	0	0	0
s_t	0	0	0	0	0	1	2	3	0	0	0	0

$$a_1 = \sum_{t=1}^4 s_t \phi(t-1) = 2 \cdot \frac{1+\sqrt{3}}{2} + 3 \cdot \frac{1-\sqrt{3}}{2} = \frac{5-\sqrt{3}}{2}.$$

For computing a_2 the sample \mathbf{s} is weighted by $\phi(t-2)$ and we get

t	-4	-3	-2	-1	0	1	2	3	4	5	6	7
$\phi(t-2)$	0	0	0	0	0	0	0	$\frac{1+\sqrt{3}}{2}$	$\frac{1-\sqrt{3}}{2}$	0	0	0
s_t	0	0	0	0	0	1	2	3	0	0	0	0

$$a_2 = \sum_{t=2}^5 s_t \phi(t-2) = \frac{3(1+\sqrt{3})}{2}.$$

For negative values of k , we use formula (8.5.16). Thus, for computing a_{-1} the average of \mathbf{s} is weighted by $\phi(t+1)$, which gives

$$a_{-1} = \sum_{t=-1}^2 s_t \phi(t+1) = \frac{1-\sqrt{3}}{2},$$

and for computing a_{-2} the average of \mathbf{s} is weighted by $\phi(t+2)$, which yields

$$a_{-2} = \sum_{t=-2}^1 s_t \phi(t+2) = 0.$$

Hence, the approximation of f is given by

$$\begin{aligned} \tilde{f}(t) &= \sum_{k=-2}^2 a_k \phi(t-k) = \frac{1-\sqrt{3}}{2} \phi(t+1) + \frac{3-\sqrt{3}}{2} \phi(t) \\ &\quad + \frac{5-\sqrt{3}}{2} \phi(t-1) + \frac{3(1+\sqrt{3})}{2} \phi(t-2). \end{aligned}$$

Note that at the edges, $\tilde{f}(0) = -\frac{1}{2} \neq 0 = s_0$, and $\tilde{f}(3) = 5 \neq 3 = s_3$, but at the remaining data $\tilde{f}(1) = 1 = s_1$ and $\tilde{f}(2) = 2 = s_2$. ■

METHOD 2. The edge effects are alleviated by extending the sample \mathbf{s} with values similar to those in the sample by reflecting them periodically in the mirrors placed at the two ends of the sample. This method will be explained by the following example.

EXAMPLE 8.5.6. Consider the sample \mathbf{s} and extend it by mirror reflection at both edges so that the extended sample becomes

$$\begin{aligned} & \{s_{-4}, s_{-3}, s_{-2}, s_{-1}; \quad s_0, s_1, s_2, s_3; \quad s_4, s_5, s_6, s_7\} \\ = & \underbrace{\{3, \quad 2, \quad 1, \quad 0\}}_{\text{reflection}}; \quad \underbrace{\{0, \quad 1, \quad 2, \quad 3\}}_{\text{data}}; \quad \underbrace{\{3, \quad 2, \quad 1, \quad 0\}}_{\text{reflection}} \end{aligned}$$

The values of a_0 , a_1 and a_2 turn out to be the same as in Example 8.5.5. We find that

$$a_2 = \sum_{t=2}^5 s_t \phi(t-2) = 3, \quad \text{and} \quad a_{-2} = \sum_{t=-2}^1 s_t \phi(t+2) = 0.$$

Thus,

$$\begin{aligned} \tilde{f}(t) &= \sum_{k=-2}^2 a_k \phi(t-k) \\ &= \frac{1-\sqrt{3}}{2} \phi(t+1) + \frac{3-\sqrt{3}}{2} \phi(t) + \frac{5-\sqrt{3}}{2} \phi(t-1) + 3\phi(t-1). \end{aligned}$$

Note that at the edges, $\tilde{f}(0) = -\frac{1}{2} \neq 0 = s_0$ and $\tilde{f}(3) = 7/2 \neq 3 = s_3$, but $\tilde{f}(1) = 1 = s_1$ and $\tilde{f}(2) = 2 = s_2$. ■

METHOD 3. The edge effects are alleviated by considering smooth periodic extensions of the data which are carried out by a mirror reflection at either end. This extension can be represented as

$$\underbrace{s_0, s_1, \dots, s_{2^n-2}, s_{2^n-1}}_{\text{data}}; \quad \underbrace{s_{2^n-1}, s_{2^n-2}, \dots, s_1, s_0}_{\text{reflection}}$$

For the computation of the last coefficients a_k that are associated with the translates $\phi(t-k)$ which overlap the right edge, we add a ‘short’ reflection. This leads to the extended data structure

$$\underbrace{s_0, s_1, \dots, s_{2^n-2}, s_{2^n-1}}_{\text{data}}; \quad \underbrace{s_{2^n-1}, s_{2^n-2}, \dots, s_1, s_0}_{\text{reflection}}; \quad \underbrace{s_0, s_1}_{\text{short reflection}}$$

The number of data entries in the 'short' reflection depends on the type of wavelets used, and is equal to the number of recursion coefficients minus two. In the case of Daubechies wavelets with the four recursion coefficients c_0, c_1, c_2, c_3 , this number is 2, and we have, therefore, added only two data entries in the 'short' reflection. Hence, the data structure with periodic smooth extension is

$$\underbrace{s_0, s_1, \dots, s_{2^n-2}, s_{2^n-1}}_{\text{data}}; \underbrace{s_{2^n}, \dots, s_{2^{n+1}-1}}_{\text{extension}}; \underbrace{s_0, s_1}_{\text{short extension}} \quad (8.5.17)$$

Note that at the right edge of the data portion of the structure in (8.5.17) the data changes by $s_{2^n-1} - s_{2^n-2}$ (which is the difference between the last two entries in the data), and this change must be equal to the change in the extension portion of the structure at the same location, which is $s_{2^n} - s_{2^n-1}$ (difference between the first entry in the extension and the last entry in the data). Thus, $s_{2^n} - s_{2^n-1} = s_{2^n-1} - s_{2^n-2}$, which gives

$$s_{2^n} = 2 s_{2^n-1} - s_{2^n-2}. \quad (8.5.18)$$

Similarly, at the left edge the data change by $s_1 - s_0$ (which is the data change in the short extension) must be equal to the change in the extension at the same location which is $s_0 - s_{2^{n+1}-1}$. Thus, $s_0 - s_{2^{n+1}-1} = s_1 - s_0$, which gives

$$s_{2^{n+1}-1} = 2 s_0 - s_1. \quad (8.5.19)$$

Now, we will determine the remaining entries $s_{2^n+1}, \dots, s_{2^{n+1}-2}$ of the extension in the structure (8.5.17) without introducing extraneous discontinuities. For this purpose we use a cubic spline consisting of a cubic polynomial $p(t)$, which has the form (see §1.7)

$$p(t) = p_0 + p_1 (t - (2^n - 1)) + p_2 (t - (2^n - 1)) (t - 2^n) + p_3 (t - (2^n - 1)) (t - 2^n) (t - (2^{n+1} - 1)), \quad (8.5.20)$$

subject to the following conditions

$$\begin{aligned} p(2^n - 1) &= s_{2^n-1}, \\ p(2^n) &= s_{2^n} = 2 s_{2^n-1} - s_{2^n-2} \quad \text{by (8.5.18),} \\ p(2^{n+1} - 1) &= s_{2^{n+1}-1} = 2 s_0 - s_1 \quad \text{by (8.5.19),} \\ p(2^{n+1}) &= s_0. \end{aligned} \quad (8.5.21)$$

The conditions (8.5.21) form the following linear system of algebraic equations in

the coefficients p_0, p_1, p_2, p_3 :

$$\begin{aligned}
 p_0 &= s_{2^n-1}, \\
 p_0 + p_1 (2^n - (2^n - 1)) &= s_{2^n} = 2 s_{2^n-1} - s_{2^n-2}, \\
 p_0 + p_1 (2^n - (2^n - 1) - (2^n - 1)) \\
 &\quad + p_2 ((2^{n+1} - 1) - (2^n - 1)) ((2^n - 1) - 2^n) = s_{2^{n+1}-1} = 2 s_0 - s_1, \\
 p_0 + p_1 (2^{n+1} - (2^n - 1)) + p_2 (2^{n+1} - (2^n - 1)) (2^{n+1} - 2^n) \\
 &\quad + p_3 (2^{n+1} - (2^n - 1)) (2^{n+1} - 2^n) (2^{n+1} - (2^{n+1} - 1)) = s_0,
 \end{aligned}$$

which simplifies to the matrix form

$$\begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ 1 & 2^n & 2^n (2^n - 1) & \\ 1 & 2^n & 2^n (2^n - 1) & 2^n (2^n + 1) \end{bmatrix} \begin{Bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{Bmatrix} = \begin{Bmatrix} s_{2^n-1} \\ 2s_{2^n-1} - s_{2^n-2} \\ 2s_0 - s_1 \\ s_0 \end{Bmatrix}.$$

This system is solved to give

$$\begin{aligned}
 p_0 &= s_{2^n-1}, \\
 p_1 &= s_{2^n-1} - s_{2^n-2}, \\
 p_2 &= \frac{2s_0 - s_1 - s_{2^n-1} - 2^n p_1}{2^n (2^n - 1)}, \\
 p_3 &= \frac{s_0 - s_{2^n-1} - (2^n + 1) p_1}{2^n (2^n + 1)} - p_2.
 \end{aligned} \tag{8.5.22}$$

Hence, to determine $s_{2^n+1}, \dots, s_{2^{n+1}-2}$ we take $s_k = p(k)$ for $2^{n+1} \leq k \leq 2^{n+1} - 2$.

EXAMPLE 8.5.7. Using the above sample \mathbf{s} , we find from (8.5.18) and (8.5.19) that $s_4 = 4$ and $s_7 = -1$, respectively. We will attach the periodic reflection to the left edge of the data, so that the extended sample (8.5.17) becomes

$$\begin{aligned}
 &\{s_{-4}, s_{-3}, s_{-2}, s_{-1}; s_0, s_1, s_2, s_3; s_4, s_5, s_6, s_7; s_0, s_1\} \\
 &= \left\{ \underbrace{4, 2, 1, -1}_{\text{periodic extension}}; \underbrace{0, 1, 2, 3}_{\text{data}}; \underbrace{4, 2, 1, -1}_{\text{reflection}}; \underbrace{0, 1}_{\text{short ext.}} \right\}
 \end{aligned}$$

where the values of s_5 and s_6 are chosen by using the mirror reflection to s_3 as 2 and 1, respectively. The values of the coefficients a_0, a_1 and a_{-1} remain the same as in Example 8.5.5, and those of a_2 and a_{-2} are computed as follows:

$$\begin{aligned}
 a_2 &= \sum_{t=2}^5 s_t \phi(t-2) = 3 \cdot \frac{1+\sqrt{3}}{2} + 4 \cdot \frac{1-\sqrt{3}}{2} = \frac{7-\sqrt{3}}{2}, \\
 a_{-2} &= \sum_{t=-2}^2 s_t \phi(t+2) = -\frac{1+\sqrt{3}}{2}.
 \end{aligned}$$

Thus,

$$\begin{aligned}\tilde{f}(t) = \sum_{k=-2}^2 a_k \phi(t-k) &= -\frac{1+\sqrt{3}}{2} \phi(t+2) + \frac{1-\sqrt{3}}{2} \phi(t+1) \\ &+ \frac{3-\sqrt{3}}{2} \phi(t) + \frac{5-\sqrt{3}}{2} \phi(t-1) + \frac{7-\sqrt{3}}{2} \phi(t-2).\end{aligned}$$

In particular, $\tilde{f}(0) = 0 = s_0$, $\tilde{f}(1) = 1 = s_1$, $\tilde{f}(2) = 2 = s_2$, $\tilde{f}(3) = 3 = s_3$, which shows that the above wavelet approximation $\tilde{f}(t)$ has practically no edge effects. ■

8.6. Fast Daubechies Transforms

The Daubechies wavelets are computed by fast transforms. We start with a sample (data) $\mathbf{s} = \{s_0, s_1, \dots, s_{2^n-2}, s_{2^n-1}\}$, which contains a number of elements equal to $N = 2^n$. If this number is not equal to radix 2, we must first extend (or shorten) the sample \mathbf{s} smoothly so that it contains 2^n elements. For this purpose we can use any of the three methods discussed in §8.3.3. The coefficients $\mathbf{a}^{(n)} = \{a_0^{(n)}, a_1^{(n)}, \dots, a_{2^n-1}^{(n)}\}$ are then used to replace the 2^n basis father wavelets defined in (8.5.13) by an equivalent combination of 2^n slower wavelets $\phi(t/2 - k)$ and 2^n slower wavelets $\psi(t/2 - 1 - k)$, so that we have

$$\tilde{f}(t) = \sum_{k=0}^{2^n-1} \left\{ a_k^{(n-1)} \phi(t/2 - k) + b_k^{(n-1)} \psi(t/2 - 1 - k) \right\}, \quad (8.6.1)$$

where the superscript $(n-1)$ indicates a slower frequency than (n) in the representation (8.5.13). The translation $t/2 \rightarrow (t/2 - 1)$ in the wavelets ψ in the representation (8.6.1) ensures that both ϕ and ψ are zero outside the same interval. For the computation of the coefficients $a_k^{(n-1)}$ and $b_k^{(n-1)}$ in (8.6.1) we use the recurrence relations

$$\begin{aligned}\phi(t) &= c_0 \phi(2t) + c_1 \phi(2t-1) + c_2 \phi(2t-2) + c_3 \phi(2t-3), \\ \psi(t) &= -c_0 \phi(2t-1) + c_1 \phi(2t) - c_2 \phi(2t+1) + c_3 \phi(2t+2),\end{aligned} \quad (8.6.2)$$

where c_0, c_1, c_2, c_3 are defined by (8.5.4). If we replace t by $t/2$ in the recurrence relations (8.6.2), we obtain

$$\begin{aligned}\phi(t/2) &= c_0 \phi(t) + c_1 \phi(t-1) + c_2 \phi(t-2) + c_3 \phi(t-3), \\ \psi(t/2) &= -c_0 \phi(t-1) + c_1 \phi(t) - c_2 \phi(t+1) + c_3 \phi(t+2).\end{aligned} \quad (8.6.3)$$

This leads to an algorithm for the Daubechies transforms, which uses the recursion (8.6.3) and yields the following system linear equations:

$$\begin{aligned}
 \phi(t/2) &= c_0 \phi(t) + c_1 \phi(t-1) + c_2 \phi(t-2) + c_3 \phi(t-3), \\
 \psi(t/2-1) &= c_3 \phi(t) - c_2 \phi(t-1) + c_1 \phi(t-2) - c_0 \phi(t-3), \\
 &\vdots \\
 \phi(t/2-k) &= c_0 \phi(t-2k) + c_1 \phi(t-1-2k) + c_2 \phi(t-2-2k) \\
 &\quad + c_3 \phi(t-3-2k), \\
 \psi(t/2-1-k) &= c_3 \phi(t-2k) - c_2 \phi(t-1-2k) + c_1 \phi(t-2-2k) \\
 &\quad - c_0 \phi(t-3-2k).
 \end{aligned} \tag{8.6.4}$$

The matrix \mathbf{D} , defined by

$$\mathbf{D} = \begin{bmatrix} c_0 & c_3 & & & \dots \\ c_1 & -c_2 & & & \dots \\ c_2 & c_1 & c_0 & c_3 & \dots \\ c_3 & -c_0 & c_1 & -c_2 & \dots \\ & & c_2 & -c_2 & \dots \\ & & c_3 & -c_0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}, \tag{8.6.5}$$

where all blank elements are zero, is known as the matrix of the change of Daubechies basis. The relations (8.5.2) hold for the inner products of the columns of the matrix \mathbf{D} . Since $\mathbf{D}^T \mathbf{D} = 2\mathbf{I}$, we have $\mathbf{D}^{-1} = \frac{1}{2} \mathbf{D}^T$, and the system (8.6.4) can be written in the matrix form by $\mathbf{D}^T \mathbf{m} = \mathbf{d}$, where

$$\begin{aligned}
 \mathbf{m} &= [\phi(t) \quad \phi(t-1) \quad \phi(t-2) \quad \phi(t-3) \quad \dots]^T, \\
 \mathbf{d} &= [\phi(t/2) \quad \psi(t/2) \quad \phi(t/2-1) \quad \psi(t/2-2) \quad \dots]^T.
 \end{aligned}$$

Thus, the wavelet transforms are computed by changing from the basis with wavelets $\phi(t-k)$ to the basis with the wavelets $\phi(t/2-k)$ and $\psi(t/2-1-k)$. This means that we can multiply the coefficients $a_k^{(n)}$ in (8.5.13) by the inverse matrix \mathbf{D}^{-1} . It requires that we read the new coefficients in a row of the type

$$\mathbf{q} = \left\{ a_0^{(n-1)}, b_0^{(n-1)}, a_1^{(n-1)}, b_1^{(n-1)}, \dots, a_{2^{n-1}-1}^{(n-1)}, b_{2^{n-1}-1}^{(n-1)} \right\},$$

which are computed in terms of the previously known elements of $\mathbf{a}^{(n)}$ by the formula

$\mathbf{q} = \frac{1}{2} \mathbf{D}^T \mathbf{a}^{(n)}$, or

$$\begin{aligned}
 & \left[a_0^{(n-1)} \quad b_0^{(n-1)} \quad a_1^{(n-1)} \quad b_1^{(n-1)} \quad \dots \quad a_{2^{n-1}-1}^{(n-1)} \quad b_{2^{n-1}-1}^{(n-1)} \right]^T \\
 &= \frac{1}{2} \begin{bmatrix} c_0 & c_1 & c_2 & c_3 & & & & & & & \\ c_3 & -c_2 & c_1 & -c_0 & & & & & & & \\ & & c_0 & c_1 & c_2 & c_3 & & & & & \\ & & c_3 & -c_2 & c_1 & -c_0 & & & & & \\ & & & & c_0 & c_1 & & & & & \\ & & & & c_3 & -c_2 & & & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & & & c_0 & c_1 & c_2 & c_3 \\ & & & & & & c_3 & -c_2 & c_1 & -c_0 \end{bmatrix} \quad (8.6.6) \\
 & \times \left[a_0^{(n)} \quad a_1^{(n)} \quad a_2^{(n)} \quad a_3^{(n)} \quad \dots \quad a_{2^{n+1}-2}^{(n)} \quad a_{2^{n+1}-1}^{(n)} \quad a_{2^{n+1}}^{(n)} \quad a_{2^{n+1}+1}^{(n)} \right]^T.
 \end{aligned}$$

This formula computes the Daubechies wavelet transforms. In this formula the coefficients $a_k^{(n)}$ are those of the wavelets $\phi(t/2 - k)$ and the coefficients $b_k^{(n)}$ those of the wavelets $\psi(t/2 - 1 - k)$. Formula (8.6.6) is used recursively for the next iterations of the coefficients $a_k^{(n)}$ and $b_k^{(n)}$ and continued until the $(N-1)$ -st iteration is computed. The details of this method can be found in Daubechies (1988, 1990), and Nievegelt (1999).

EXAMPLE 8.6.1. For $N = 2^2 = 4$ ($n = 2$), let the sample (data) be $\mathbf{s} = \{0, 1, 2, 3\}$.

STEP 1. A periodic extension of this data gives

$$\underbrace{0, \quad 1, \quad 2, \quad 3;}_{\text{data}} \quad \underbrace{4, \quad 2, \quad 1, \quad -1;}_{\text{extension}} \quad \underbrace{0, \quad 1}_{\text{short extension}}$$

(see Example 8.5.7).

STEP 2. Compute the coefficients $a_k^{(n)}$ for $k = 0, 1, \dots, 7 = 2^n - 1$, as in Example 8.5.7, and obtain

$$\begin{aligned}
 \tilde{f}(t) &= \frac{3 - \sqrt{3}}{2} \phi(t) + \frac{5 - \sqrt{3}}{2} \phi(t-1) + \frac{7 - \sqrt{3}}{2} \phi(t-2) \\
 &\quad + \left(3 + \sqrt{3}\right) \phi(t-3) + \frac{3 + \sqrt{3}}{2} \phi(t-4) + \sqrt{3} \phi(t-5) \\
 &\quad - \frac{1 + \sqrt{3}}{2} \phi(t-6) + \frac{1 - \sqrt{3}}{2} \phi(t-7).
 \end{aligned}$$

STEP 3. Use formula (8.6.6) recursively to compute

$$a_0^{(n-1)}, a_1^{(n-1)}, a_2^{(n-1)}, a_3^{(n-1)}, \quad \text{and} \quad b_0^{(n-1)}, b_1^{(n-1)}, b_2^{(n-1)}, b_3^{(n-1)},$$

which gives

$$\{a_0^{(n-1)}, a_1^{(n-1)}, a_2^{(n-1)}, a_3^{(n-1)}\} = \left\{ \frac{18 - 5\sqrt{3}}{8}, \frac{7 + 5\sqrt{3}}{4}, \frac{8 + 3\sqrt{3}}{8}, 1 - \sqrt{3} \right\},$$

$$\{b_0^{(n-1)}, b_1^{(n-1)}, b_2^{(n-1)}, b_3^{(n-1)}\} = \left\{ -\frac{3}{8}, \frac{1 - \sqrt{3}}{4}, \frac{1 - 6\sqrt{3}}{8}, 0 \right\}.$$

Using formula (8.6.6) with the new recursive data

$$\{a_0^{(n-1)}, a_1^{(n-1)}, a_2^{(n-1)}, a_3^{(n-1)}, b_0^{(n-1)}, b_1^{(n-1)}, \dots\},$$

the next iteration gives

$$\{a_0^{(n-2)}, a_1^{(n-2)}\} = \left\{ \frac{61 + 21\sqrt{3}}{32}, \frac{35 - 21\sqrt{3}}{32} \right\},$$

$$\{b_0^{(n-2)}, b_1^{(n-2)}\} = \left\{ \frac{35 - 11\sqrt{3}}{32}, \frac{-27 + 3\sqrt{3}}{32} \right\}.$$

The next, and final, iteration with the known previous data

$$\{a_0^{(n-2)}, a_1^{(n-2)}, b_0^{(n-2)}, b_1^{(n-2)}, \dots\},$$

yields

$$\{a_0^{(n-3)}\} = \left\{ \frac{3}{2} \right\}, \quad \{b_0^{(n-3)}\} = \left\{ \frac{13 + 21\sqrt{3}}{32} \right\}.$$

Hence, we obtain

$$\begin{aligned} \tilde{f}(t) &= \sum_{k=0}^7 a_k \phi(t - k) \\ &= \sum_{k=0}^3 \left\{ a_k^{(n-1)} \phi(t/2 - 2k) + b_k^{(n-1)} \psi(t/2 - 1 - 2k) \right\} \\ &= \sum_{k=0}^1 \left\{ a_k^{(n-2)} \phi(t/4 - 4k) + b_k^{(n-2)} \psi(t/4 - 1 - 4k) \right\} \\ &\quad + \sum_{k=0}^3 b_k^{(n-1)} \psi(t/2 - 1 - 2k) \\ &= a_0^{(n-3)} \phi(t/8) + b_0^{(n-3)} \phi(t/8) \\ &\quad + \sum_{k=0}^1 c_k^{(n-2)} \psi(t/4 - 1 - k) + \sum_{k=0}^3 b_k^{(n-1)} \psi(t/2 - 1 - 2k) \end{aligned}$$

$$\begin{aligned}
&= \frac{3}{2} \phi(t/8) + \frac{13 + 21\sqrt{3}}{32} \psi(t/8 - 1) + \frac{35 - 11\sqrt{3}}{32} \psi(t/4 - 1) \\
&\quad + \frac{-27 + 3\sqrt{3}}{32} \psi(t/4 - 5) - \frac{3}{8} \psi(t/2 - 1) + \frac{1 - 3\sqrt{3}}{4} \psi(t/2 - 3) \\
&\quad + \frac{1 - 6\sqrt{3}}{8} \psi(t/2 - 5) + 0 \cdot \psi(t/2 - 7). \blacksquare
\end{aligned} \tag{8.6.7}$$

9

Integral Equations

We will confine to numerical solutions of Fredholm integral equations that involve orthogonal polynomials and application of quadrature rules. Details about these and other types of integral equations are available, e.g., in Atkinson (1976), Baker (1978), Porter and Stirling (1993), and Kythe and Puri (2002). Definitions of various technical terms and classification of integral equations can be found in most books on the subject. We have followed the notation used in Baker (1978), Porter and Stirling (1993), and Kythe and Puri (2002).

9.1. Nyström System

For an integral equation of a single real variable, the unknown function will be denoted by $\phi(x)$, the kernel of the equation by $k(x, s)$, and the free term (assumed known) by $f(x)$. The kernel and the free term are, in general, complex-valued functions of a real variable. We will write Fredholm equations of the first and second kinds in short by FK1 and FK2, respectively. Let $\lambda \neq 0$ be a (complex) numerical parameter, usually denoting the eigenvalues of the kernel. The terms ‘eigenvalues’ and ‘characteristic values’ are generally used interchangeably in eigenvalue problems, but we will keep the distinction between these two terms and denote eigenvalues by λ and characteristic values by μ , such that $\mu = 1/\lambda$. The Fredholm equations of the first kind (FK1) are defined by

$$\int_a^b k(x, s)\phi(s) ds = f(x), \quad a \leq x \leq b, \quad (9.1.1)$$

and of the second kind (FK2) by

$$\phi(x) = f(x) + \lambda \int_a^b k(x, s) \phi(s) ds, \quad a \leq x \leq b. \quad (9.1.2)$$

If $f(x) = 0$ in $[a, b]$, Fredholm equations are said to be *homogeneous*; otherwise they are inhomogeneous. The superposition principle applies to linear and homogeneous equations only. Fredholm equations are *linear* integral equations. It is assumed that the functions $\phi(x)$ and $f(x)$ belong to the class $L_2[a, b]$, and the kernel $k(x, s)$ is continuous on the square $S = \{(x, s) : x, s \in [a, b] \times [a, b]\}$, or is such that $k(x, s)$ is square-integrable on S , i.e.,

$$\int_a^b \int_a^b k^2(x, s) dx ds = B^2 < \infty \quad \text{on } S,$$

and that $k(x, s) \equiv 0$ for $s > x$. In terms of the integral operator K defined by

$$(K\phi)(x) = \int_a^b k(x, s) \phi(s) ds, \quad a \leq x \leq b,$$

the integral equations (9.1.1)–(9.1.2) are expressed in terms of the operator K as $K\phi = f$, and $\phi = f + \lambda K\phi$, respectively.

A quadrature rule for computing the integral $I_a^b(f)$ of the form (2.6.1) is used to compute the integral occurring in Eq (9.1.1). We obtain

$$\int_a^b k(x, s) \phi(s) ds = \sum_{j=0}^n w_j k(x, s_j) \tilde{\phi}(s_j),$$

where $\tilde{\phi}$ denotes an approximate value of ϕ , and the integral equation leads to the eigenvalue problem

$$\sum_{j=0}^n w_j k(x, s_j) \tilde{\phi}(s_j) = \tilde{\mu} \tilde{\phi}(x), \quad a \leq x \leq b, \quad (9.1.3)$$

whose solution gives an approximate eigenvalue $\tilde{\lambda}$ and an associated eigenfunction $\tilde{\phi}(x)$. The problem (9.1.3) is solved by the *Nyström method*, which is as follows: Set $x = x_i, i = 0, 1, \dots, n$, in (9.1.3), which yields the system of $(n + 1)$ algebraic equations

$$\sum_{j=0}^n w_j k(x_i, s_j) \tilde{\phi}(s_j) = \tilde{\mu} \tilde{\phi}(x_i), \quad i = 0, 1, \dots, n, \quad (9.1.4)$$

where the points x_i are called the Nyström points, $a \leq x_i \leq b$, and s_j are the nodes. Setting $\mathbf{k} = [k(x_i, s_j)]$, $\tilde{\Phi} = [\tilde{\phi}(x_0), \tilde{\phi}(x_1), \dots, \tilde{\phi}(x_n)]^T$, and $\mathbf{D} = \text{diag}(w_0, w_1, \dots, w_n)$, the system (9.1.4) becomes the matrix eigenvalue problem

$$\mathbf{kD}\tilde{\Phi} = \tilde{\mu}\tilde{\Phi}, \quad (9.1.5)$$

which, when solved, yields $(n+1)$ eigenvalues $\tilde{\lambda}_m = 1/\tilde{\mu}_m$, $m = 0, 1, \dots, n$, and the associated eigenfunctions $\tilde{\phi}_m$. Note that the solution of the system (9.1.4) or (9.1.5) depends on the choice of the values of x_i and that different choices of x_i and s_j generate different solutions, where the choice of s_j becomes fixed depending on the quadrature rule used. The problem of optimizing the choice of the Nyström points x_i that will yield the best solution is still open. Although it is not necessary to choose the Nyström points x_i same as the nodes s_j , $i, j = 0, 1, \dots, n$, it is usually done so, except in the case when the kernel is not defined at $x = s$ or becomes unbounded there. With this choice the determinant of the matrix \mathbf{k} in (9.1.5) is symmetric if the kernel is symmetric. If $\tilde{\mu}_m \neq 0$, the eigenvectors $\tilde{\phi}_m$ may be extended to a function $\tilde{\phi}_m(x)$ by substituting it in Eq (9.1.3), that is,

$$\tilde{\phi}_m(x) = \tilde{\lambda}_m \sum_{j=0}^n w_j k(x, s_j) \tilde{\phi}_m(s_j). \quad (9.1.6)$$

The function $\tilde{\phi}_m(x)$ is called the *Nyström extension* of the eigenvector $\tilde{\phi}_m$.

EXAMPLE 9.1.1. Consider the eigenvalue problem (Baker 1978, p.171)

$$\int_0^1 k(x, s)\phi(s) ds = \mu\phi(x), \quad 0 \leq x \leq 1,$$

with a symmetric kernel defined for $0 \leq x \leq s \leq 1$ by

$$k(x, s) = \begin{cases} \frac{x}{2}(2-s) & \text{if } x \leq s, \\ \frac{s}{2}(2-x) & \text{if } x \geq s. \end{cases}$$

The exact eigenvalues are the roots of the equation $\sqrt{\lambda} + \tan \sqrt{\lambda} = 0$, with the corresponding eigenfunctions $\phi(x) = \sin(\sqrt{\lambda}x)$. Thus, the first four exact eigenvalues are $\mu_1 = 0.24296$, $\mu_2 = 0.041426$, $\mu_3 = 0.015709$. Using a 3-point trapezoidal rule on $[0, 1]$ we have $Q(F) = 0.25 F(0) + 0.5 F(0.5) + 0.25 F(1)$, and choosing $x_0 = s_0 = 0$, $x_1 = s_1 = 1/2$, $x_2 = s_2 = 1$, we find that

$$\mathbf{kD} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 3/16 & 1/16 \\ 0 & 1/8 & 1/8 \end{pmatrix},$$

so that the solution of the system (9.1.5) reduces to solving $\mathbf{kD} - \mu = 0$, which gives the approximate characteristic values as $\tilde{\mu}_1 = 1/4$, $\tilde{\mu}_2 = 1/16$, and $\tilde{\mu}_3 = 0$. Note

that the eigenvector corresponding to μ_3 is $\tilde{\phi}_3 = [1, 0, 0]^T$. But since $\tilde{\mu}_3 = 0$, we cannot use the Nyström extension formula (9.1.4) to extend the eigenvector $\tilde{\phi}_3$ to a function $\tilde{\phi}_3(x)$. Even if we choose different values for x_0 , say, $x_0 = 1/10$ or $1/100$, we find the same characteristic values as above. If instead of the 3-point trapezoidal rule we use the 4-point trapezoidal, or Simpson's 3/8 rule, the situation remains the same; thus, in the case of the 4-point trapezoidal rule we find that $\tilde{\mu}_1 = 0.0138889$, $\tilde{\mu}_2 = 0.123069$, $\tilde{\mu}_3 = 0.250787$, and $\tilde{\mu}_4 = 0$, whereas in the case of Simpson's 3/8 rule we get $\tilde{\mu}_1 = 0.0245766$, $\tilde{\mu}_2 = 0.0514826$, $\tilde{\mu}_3 = 0.257274$, and $\tilde{\phi}_4 = 0$ (see [nystrom1.nb](#) on the CD-R for computational details), and again, we cannot use the Nyström extension formula (9.1.4) to extend the eigenvector $\tilde{\phi}_4$ to a function $\tilde{\phi}_4(x)$. Thus, to extend an eigenvector $\tilde{\phi}_m$ to an eigenfunction $\tilde{\phi}_m(x)$ by the formula (9.1.6), it is necessary that the corresponding characteristic value $\tilde{\mu}_m$ be nonzero. ■

EXAMPLE 9.1.2. Consider the eigenvalue problem with the kernel defined on $(0, 1]$ by

$$k(x, s) = \begin{cases} -\sqrt{xs} \ln s, & x \leq s, \\ -\sqrt{xs} \ln x, & x \geq s. \end{cases}$$

Since the kernel is undefined at $x = 0$, we shall use a 3-point trapezoidal rule by choosing $x_0 = s_0 = 0$, $x_1 = s_1 = 1/2$, and $x_2 = s_2 = 1$. Then we have

$$\mathbf{k} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (\ln 2)/2 & 0 \\ 0 & -(\ln 2)/\sqrt{2} & 0 \end{pmatrix},$$

and the solution of the system (9.1.5) gives $\tilde{\mu}_1 = 0.173287$, $\tilde{\mu}_2 = \tilde{\mu}_3 = 0$. If, in view of the fact that the kernel is not defined at $x = 0$, we opt to choose the Nyström points as $x_0 = 1/100$, $x_1 = 1/2$, and $x_2 = 1$, we still get the same values for $\tilde{\mu}_1$, $\tilde{\mu}_2$ and $\tilde{\mu}_3$. Thus, it makes no difference if we choose a different Nyström point x_0 . In fact, the point x_0 can be any point in $(0, 1/2)$. Hence, for this problem we cannot extend the eigenvectors $\tilde{\phi}_2$ and $\tilde{\phi}_3$. For computational details see [nystrom2.nb](#) on the CD-R. ■

An FK2 of the form $(\mu I - K)\phi = f$, $a \leq x \leq b$, where $k \in C[a, b]$ can be approximated by

$$\mu \tilde{\phi}(x) - \sum_{j=1}^n w_j k(x, s_j) \tilde{\phi}(s_j) = f(x), \quad a \leq x \leq b. \quad (9.1.7)$$

By replacing x by the Nyström points x_i , $i = 1, \dots, n$, we obtain a linear system

$$\mu \tilde{\phi}(x_i) - \sum_{j=1}^n w_j k(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad i = 1, \dots, n, \quad (9.1.8)$$

or in matrix form

$$(\mu \mathbf{I} - \mathbf{kD}) \tilde{\Phi} = \mathbf{f},$$

where \mathbf{I} is the identity matrix. Each solution $\tilde{\phi}(x)$ of (9.1.7) leads to the solution $\{\tilde{\phi}(x_1), \dots, \phi(x_n)\}$ of the system (9.1.8). Also, if the two solutions of (9.1.7) match at the points s_1, \dots, s_n , then they match at all points of $[a, b]$.

EXAMPLE 9.1.3. Consider the FK2

$$\phi(x) + \int_0^1 \sqrt{xs} \phi(s) ds = \sqrt{x}, \quad 0 \leq x \leq 1,$$

whose exact solution is $\phi(x) = 2\sqrt{x}/3$. We use the 3-point trapezoidal rule with $x_0 = s_0 = 0$, $x_1 = s_1 = 1/2$, and $x_2 = s_2 = 1$, and solve the system $(\mathbf{I} + \mathbf{kD}) \tilde{\Phi} = \mathbf{f}$. The results are $\tilde{\phi}_1 = 0$, $\tilde{\phi}_2 = 0.471405$ and $\tilde{\phi}_3 = 0.666667$, which match the exact solution. For computational details see [nystrom3.nb](#) on the CD-R. ■

On certain guidelines for using the Nyström method, see [Kythe and Puri](#) (2002, p.27).

9.2. Integral Equations of the First Kind

Fredholm equations of the first kind, defined by (9.1.1), are inherently ill-posed (see [Groetsch](#) 1984, [Kress](#) 1989, [Hansen](#) 1992, [Golberg and Chen](#) 1997, [Kythe and Puri](#) 2002), and therefore their numerical solution is difficult. The ill-posedness of an FK1 generally results in unstable solutions and a small error can lead to an unbounded error. We pointed out this ill-posedness problem in [Chapter 7](#) for the inverse Laplace transform problem, since Eq (7.1.2) is basically an FK1. Another source of ill-posedness is the Riemann-Lebesgue lemma. Also, if both $\phi(x)$ and $k(x, s)$ are continuous but $f(x)$ is not, then Eq (9.1.1) is not solvable.

9.2.1. Use of Numerical Quadrature. Partition the interval $[a, b]$ into n equal parts of length $h = (b - a)/n$, and approximate Eq (9.1.1) by

$$f(x) \approx \sum_{j=1}^n k(x, s_j) \phi(s_j) h,$$

which after setting $x = x_1, x_2, \dots, x_n$ gives

$$f_i = \sum_{j=1}^n k_{ij} \phi_j, \quad i = 1, 2, \dots, n,$$

where $f_i = f(x_i)$, $k_{ij} = k(x_i, s_j) h$, and $\phi_j = \phi(s_j)$, which form a system of n equations in n unknowns ϕ_i . However, the solution so obtained depends on the choice of the values of x , and different choices of x yield different solutions. We may

choose the nodes s_j the same as the Nyström points x_i , but it is not always possible, e.g., in the case of a kernel that is not defined at $x = s$ or becomes unbounded there. The quadrature method for FK1 is found to be very unsatisfactory as the following examples show.

EXAMPLE 9.2.1. Consider the FK1 with $k(x, s) = \begin{cases} x(1-s) & \text{if } x \leq s, \\ s(1-x) & \text{if } x \geq s, \end{cases}$ defined on $[0, 1]$. First, we apply the repeated trapezoidal rule by choosing $x_i = s_i = ih$, $h = 1/n$, for $i = 0, 1, \dots, n$. Now, since $k(0, s) = k(1, s) = k(x, 0) = k(x, 1) = 0$ for $0 \leq x \leq s \leq 1$, we obtain the system

$$h \sum_{j=1}^n k(ih, jh) \tilde{\phi}(jh) = f(ih), \quad i = 0, 1, \dots, n, \quad (9.2.1)$$

where $f(ih) = f(0) = 0$ for $i = 0$ and $f(ih) = f(1) = 0$ for $i = n$. But this system fails to compute the values $\tilde{\phi}(0)$ and $\tilde{\phi}(1)$. Suppose that $f(0) = f(1) = 0$; otherwise this method yields no solution. Since

$$h k(ih, jh) = \begin{cases} ih^2(1-jh) & \text{if } i \leq j, \\ jh^2(1-ih) & \text{if } i \geq j, \end{cases}$$

we obtain the system (9.2.1) yields the matrix equation $\tilde{\Phi} = \mathbf{A} \mathbf{f}$, where

$$\tilde{\Phi} = [\tilde{\phi}(h) \quad \tilde{\phi}(2h) \quad \tilde{\phi}(3h) \quad \dots \quad \tilde{\phi}(1-2h) \quad \tilde{\phi}(1-h)],$$

$$\mathbf{A} = -\frac{1}{h^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ & 1 & -2 & 1 & & \\ & & 1 & -2 & 1 & \\ & & \dots & \dots & \dots & \dots \\ & & & & & 1 \\ & & & & 1 & -2 \end{bmatrix},$$

$$\mathbf{f} = \begin{Bmatrix} f(h) \\ f(2h) \\ f(3h) \\ \vdots \\ f(1-2h) \\ f(1-h) \end{Bmatrix},$$

$$\tilde{\phi}(ih) = -\frac{1}{h^2} [f((i-1)h) - 2f(ih) + f((i+1)h)], \quad f(0) = 0, \quad f(1) = 0.$$

Thus, $\tilde{\phi}(ih) \approx -f''(ih)$, where it is assumed that $f \in C^2[0, 1]$. This shows that the trapezoidal rule is satisfactory only if $f(0) = 0 = f(1)$, and computation of the derivative $f''(ih)$ is unstable due to roundoff errors in $f(x)$.

Next, if we use the repeated Simpson’s rule, we obtain a similar system of equations as $\tilde{\Phi} = \mathbf{A} \mathbf{f}$ except that the vector $\tilde{\Phi}$ is replaced by

$$\tilde{\Phi} \equiv \left[\frac{4}{3} \tilde{\phi}(h) \quad \frac{2}{3} \tilde{\phi}(2h) \quad \frac{4}{3} \tilde{\phi}(3h) \quad \dots \quad \frac{2}{3} \tilde{\phi}(1-2h) \quad \frac{4}{3} \tilde{\phi}(1-h) \right]^T,$$

with $h = 1/n$ and $n = 2m$. Then

$$\tilde{\phi}(ih) \rightarrow \begin{cases} -\frac{3}{4} f''(ih) & \text{if } i \text{ is odd,} \\ -\frac{3}{2} f''(ih) & \text{if } i \text{ is even,} \end{cases}$$

which gives inaccurate results for $\tilde{\Phi}$. Also, if $k(x_i, s_j) = 0$ for some i and all s_j , or if $k(x_i, s_j) = 0$ for some j and all x_i , we may run into a different kind of problem in that $\det(\mathbf{k}) = 0$. Moreover, by making an ‘unsuitable’ choice of the Nyström points x_i or the nodes s_j , the matrix \mathbf{k} may become almost singular or ill-conditioned, which leads to unacceptable solutions.

Finally, if we use Gaussian quadrature rules, then for each point x we can write

$$f(x) = \sum_{j=1}^n w_j k(x, s_j) \phi(s_j),$$

where w_j are weights connected to the particular Gaussian rule used. As before, this would generate a system of n equations in n unknowns $\phi(s_j)$. If the determinant of the system is nonsingular, we find the approximate values $\tilde{\phi}(x)$ of $\phi(x)$ at the n nodes in $[a, b]$. In general, it is convenient to change the interval to $[0, 1]$ by a linear transformation, provided a and b are finite. However, in most cases the matrix of the system is ill-conditioned and this method is not very successful as the following example shows.

EXAMPLE 9.2.2. Consider the FK1 of Example 9.2.1. The minimum norm solution of the equation is $\phi(x) = 6x$. Using a four-point Gauss-Chebyshev rule the computed values of $\tilde{\phi}(x)$, given in Table 9.2.2, are compared with those obtained by Kondo (1991). Obviously, none of these values is acceptable. ■

Table 9.2.2

x	$\tilde{\phi}(x)$	$\tilde{\phi}(x)$ (Kondo)
0.102673	6.94159	202.685303
0.406204	−4.59716	−182.9258184
0.593769	−1.61587	73.620687
0.897327	11.2714	19.482761

Although not always successful, quadrature methods should not be totally discarded; they sometimes do yield acceptable results (see [Baker 1978](#), [Caldwell 1994](#)).

9.2.2. Regularization Methods. There are eight regularization methods which together with the methods discussed in [Chapter 7](#) and certain quadrature rules help in obtaining approximate solutions of FK1, and provide useful methods for computing $\tilde{\Phi}$. These methods are as follows.

9.2.2(a) Phillips' Method. (Phillips 1962) If the function $f(x)$ in Eq (9.1.1) is not known accurately, an error $\epsilon(x)$ may occur in its evaluation. Thus, we solve the modified equation

$$\int_a^b k(x, s)\phi(s) ds = f(x) + \epsilon(x), \quad (9.2.2)$$

where $\epsilon(x)$ is an arbitrary function except for a condition on its size, and obtain a family \mathcal{F} of its solutions. But to determine the true solution, some additional information is needed. Assuming that ϕ is a reasonably smooth function, we choose as solution a function from the family \mathcal{F} , which is the smoothest in some sense. We may use the condition that the function ϕ must have a piecewise continuous second derivative, i.e.,

$$\int_a^b \phi_s''(x) dx = \min_{\phi \in \mathcal{F}} \int_a^b \phi''(x) dx. \quad (9.2.3)$$

We partition the interval $[a, b]$ into n equal subintervals at the points $a = s_0 < s_1 < s_2 < \dots < s_n = b$, $n(s_i - s_{i-1}) = b - a$, and replace Eq (9.2.2) by the linear system

$$\sum_{j=0}^n w_j k_{ij} \phi_j = f_i + \epsilon_i, \quad i = 0, 1, \dots, n, \quad (9.2.4)$$

where $\phi_j = \phi(s_j)$, $f_i = f(x_i)$, $\epsilon_i = \epsilon(x_i)$, $k_{ij} = k(x_i, s_j)$, and w_j denotes the weights for the quadrature rule used, and on $\epsilon(x)$ we impose the condition that

$$\sum_{i=0}^n \epsilon_i^2 = e^2, \quad (9.2.5)$$

where e is a constant. Another choice is the condition $\sum_{i=0}^n p_i \epsilon_i^2 = e^2$, $p_i \geq 0$, or Eq (9.2.3) can be expressed in terms of the second difference by

$$\sum_{i=0}^n (\phi_{i+1}^s - 2\phi_i^s + \phi_{i-1}^s)^2 = \min_{\phi \in \mathcal{F}^*} \sum_{i=0}^n (\phi_{i+1} - 2\phi_i + \phi_{i-1})^2, \quad (9.2.6)$$

where $\Phi^s = [\phi_0^s, \phi_1^s, \dots, \phi_n^s]^T$, and \mathcal{F}^* denotes a set of functions that satisfy (9.2.4) and (9.2.5). It is assumed in (9.2.6) that ϕ vanishes outside the interval $[a, b]$, and thus,

$\phi_{-1} = \phi_{n+1} = 0$. If we introduce the matrices $\mathbf{A} = (w_j k_{ij})$, where $\mathbf{A}^{-1} = (\alpha_{ij})$, Eq (9.2.4) is written as $\mathbf{A} \Phi = \mathbf{f} + \epsilon$, which implies that

$$\Phi = \mathbf{A}^{-1}(\mathbf{f} + \epsilon) = \mathbf{A}^{-1}\mathbf{f} + \mathbf{A}^{-1}\epsilon. \quad (9.2.7)$$

Thus, the functions ϕ_j are linear in ϵ_i and

$$\frac{\partial \phi_i}{\partial \epsilon_j} = \alpha_{ij}, \quad i, j = 0, 1, \dots, n. \quad (9.2.8)$$

Using (9.2.5) and (9.2.8) and the constraint (9.2.5), we find the conditions which ϕ_j must satisfy are

$$\sum_{j=0}^n (\phi_{j+1}^s - 2\phi_j^s + \phi_{j-1}^s) (\alpha_{i+1,j} - 2\alpha_{ij} + \alpha_{i-1,j}) + \gamma^{-1} \epsilon_i = 0, \quad (9.2.9)$$

for $i = 0, 1, \dots, n$, together with the constraint (9.2.5), where γ^{-1} is the Lagrange multiplier. Since both ϵ_i and γ are unknown, we consider the problem as that of finding the vector \mathbf{f}^s satisfying (9.2.4) by minimizing

$$\gamma \sum_{j=0}^n (\phi_{j+1}^s - 2\phi_j^s + \phi_{j-1}^s)^2 + \sum_{i=0}^n \epsilon_i^2, \quad (9.2.10)$$

for a given constant value of γ which is nonnegative in view of (9.2.9). For $\gamma = 0$ the problem reduces to that of solving $\mathbf{A} \Phi = \mathbf{f}$. For $\gamma > 0$ Eq (9.2.9) can be reduced to

$$\gamma \mathbf{B} \Phi^s = \epsilon, \quad (9.2.11)$$

where

$$\begin{aligned} \beta_{mj} &= \alpha_{m-2,j} - 4\alpha_{m-1,j} + \alpha_{m,j} - 4\alpha_{m+1,j} + \alpha_{m+2,j}, \\ \alpha_{-2,j} &= -\alpha_{0,j}, \quad \alpha_{-1,j} = 0 = \alpha_{n+1,j}, \\ \alpha_{n+2,j} &= \alpha_{n,j}, \quad j = 0, 1, \dots, n, \end{aligned}$$

Substituting (9.2.11) into Eq (9.2.7), we find that

$$\Phi^s = (\mathbf{A} + \gamma \mathbf{B})^{-1} \mathbf{f}, \quad \epsilon = -\gamma \mathbf{B} \Phi^s.$$

The choice of γ is the only question left to answer. Since increasing γ improves the smoothness, we must choose the largest γ that keeps ϵ below its preassigned value. In practice, the solution for a few values of γ is enough to determine the best solution.

EXAMPLE 9.2.3. (Phillips 1962, and Baker et al. 1964) Consider the integral equation

$$\int_{-6}^6 k(x-s)\phi(s)ds = f(x),$$

where

$$k(z) = \begin{cases} \cos \frac{\pi z}{3} & \text{if } |z| \leq 3, \\ 0 & \text{if } |z| > 3, \end{cases}$$
$$f(x) = (6 - |x|)\left(1 + \frac{1}{2} \cos \frac{\pi x}{3}\right) + \frac{9}{\pi} \sin \frac{\pi |x|}{3}.$$

The exact solution of this equation is $\phi(x) = k(x)$. The values of $\tilde{\phi}(x)$ obtained by using the trapezoidal and Simpson’s rules are presented in Table 9.2.3. Although these results obtained using Mathematica are somewhat different from those by Phillips, they bear out Phillips’ main conclusions that a well-designed regularization improves the accuracy of the solution. The unregularized results using trapezoidal rule were quite accurate. For computational details, see [phillips.nb](#) on the CD-R. ■

Table 9.2.3.

x	0.0	± 1.0	± 2.0	± 3.0	± 4.0	± 5.0	± 6.0
$\tilde{\phi}(x)$ (Trapezoidal)	1.962	1.538	0.462	0.019	0.0	0.0	0.0
$\tilde{\phi}(x)$ (Simpson)	2.943	1.154	0.693	0.014	0.0	0.0	0.0
$\phi(x)$ (Exact)	2.000	1.500	0.500	0.0	0.0	0.0	0.0
$\tilde{\phi}(x)$, $\gamma = 0.0011$	2.357	1.404	0.387	0.078	−0.033	0.004	−0.009
$\tilde{\phi}(x)$, $\gamma = 0.011$	2.098	1.476	0.449	0.006	0.041	0.011	−0.069
$\tilde{\phi}(x)$, $\gamma = 0.03$	2.031	1.486	0.489	−0.006	0.023	0.019	−0.060
$\tilde{\phi}(x)$, $\gamma = 0.1$	1.950	1.488	0.557	−0.010	−0.029	0.026	−0.012
$\tilde{\phi}(x)$, $\gamma = 0.5$	1.846	1.477	0.646	0.012	−0.091	0.017	0.037
$\tilde{\phi}(x)$, $\gamma = 1.0$	1.800	1.463	0.679	0.041	−0.100	−0.003	0.031

9.2.2(b) Twomey’s Method. Twomey (1963) suggested a simplification of the Phillips’ method as follows: Instead of minimizing the expression (9.2.10) with respect to ϵ_i , minimize it with respect to ϕ_j . Then differentiating (9.2.10) with respect to ϕ_j and taking a_{ij} as the elements of the matrix **A**, we get

$$\mathbf{A}^T \boldsymbol{\epsilon} + \gamma \mathbf{H} \boldsymbol{\Phi} = 0,$$

(9.2.12)

where **H** is the matrix

$$\mathbf{H} = \begin{pmatrix} 1 & -2 & 1 & 0 & 0 & \cdot & \cdot & \cdot \\ -2 & 5 & 4 & 1 & 0 & \cdot & \cdot & \cdot \\ 1 & 4 & 6 & -4 & 1 & 0 & \cdot & \cdot \\ 0 & 1 & -4 & 6 & -4 & 1 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

Eliminating ϵ from (9.2.7) and (9.2.12), we obtain

$$\mathbf{A} \Phi + \gamma \mathbf{B} \Phi = \mathbf{f},$$

where $\mathbf{B} = (\mathbf{A}^{-1})^T \mathbf{H}$. Note that the above equation has the same solution as given by Phillips (1962). Twomey (1963) points out that one can use higher-order regularization by minimizing the third difference rather than the second difference. He also gives an alternate form of the matrix \mathbf{H} . But these techniques will work only if the matrix \mathbf{A} is invertible. In fact, depending on the order of the expected smoothness, one can minimize $\|L\phi\|$ in any norm, where L is a linear differential operator.

EXAMPLE 9.2.4. We solve Example 9.2.3 by using Twomy’s regularization scheme. The results are given in Table 9.2.4 for the values of $x \in [-3, 3]$; the values of $x = \pm 4, \pm 5, \pm 6$ are not given since they are found to be close to zero and are, therefore, not significant. Also, the values for different values of γ are not symmetric about $x = 0$. For computational details, see [phillips.nb](#) on the CD-R.

Table 9.2.4.

x	$\gamma = 0.0011$	$\gamma = 0.011$	$\gamma = 0.03$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
-3	0.0774	-0.0031	-0.0172	-0.0135	0.1889	0.0450
-2	0.3821	0.4640	0.5052	0.5628	0.6514	0.6824
-1	1.4069	1.4798	1.4897	1.4879	1.4695	1.4549
0	2.3563	2.0792	2.0102	1.9402	1.8414	1.8008
1	1.3996	1.4764	1.4882	1.4942	1.4913	1.4832
2	0.3951	0.4723	0.5157	0.5720	0.6557	0.6816
3	0.0802	-0.0030	-0.0207	-0.0266	-0.0163	-0.0055 ■

Essah and Delves (1989) have developed a cross-validation scheme to automatically set two regularization parameters (constraints) introduced into the solution of an FK1 by using a Chebyshev series method (see [Kythe and Puri 2002](#), p. 338, for details). In view of the use of Laguerre polynomials in Weeks’ method (§7.2.5(c)), the Gauss-Laguerre rule (§3.2.3) can be very helpful in Twomey’s method, but no approach has been made in this direction.

9.2.2(c) Caldwell’s Method. Caldwell (1994) compares different methods for the numerical solution of FK1. He considers the usual quadrature methods and finds that classical quadrature methods do not give good results in general but can be useful for special problems. He proposes a modification of the quadrature method by replacing the FK1 (9.1.1) by

$$\phi(s_i) \int_a^b k(s_i, s) \, ds + \sum_{j=0, j \neq i}^n \omega_j k(s_i, s_j) [f(s_j) - f(s_i)] = f(s_i).$$

Clearly, by this method one should be able to compute $\phi(s_i) \int_a^b k(s_i, s) ds$ to a high degree of accuracy. However, Caldwell comments that this approach suffers from the same defect as quadrature methods but might be better in some cases. In this approach, instead of approximating $k(x, s)\phi(s)$, one approximates only $\phi(s)$. To avoid computation of the weights for each x , he proposes using the midpoint rule. This method is based on the assumption $\phi(x)$ is slowly varying and in each subinterval (s_j, s_{j+1}) it can be assumed to be constant equal to $\phi(s_{jm})$, where s_{jm} is the middle point of the subinterval. The method yields the following equation:

$$\sum_{j=0}^{n-1} \phi(s_{jm}) \int_{s_j}^{s_{j+1}} k(s_i, s) ds = f(s_i).$$

This method is particularly useful when $k(x, s)$ is badly behaved but $\phi(x)$ is not.

Caldwell also considers the simplest form of the regularization method, which is as follows: Consider an FK2 of the form

$$\int_a^b k(x, s)\phi_\epsilon(s) ds + \epsilon\phi_\epsilon(x) = f(x),$$

where ϵ is a small, positive parameter. Then obtain a sequence of solutions $\phi_\epsilon(x)$ for some suitable values of ϵ , and extrapolate the results to $\epsilon \rightarrow 0$. Thus, $\lim_{\epsilon \rightarrow 0} \|\phi_\epsilon(x) - \phi(x)\| = 0$ in the L_2 -norm, but this convergence is not uniform. Lastly, his iteration method for a symmetric kernel has the form

$$\Phi_{(n+1)} = \Phi_{(n)} + \alpha (\mathbf{f} - \mathbf{k} \Phi_{(n)}), \quad \Phi_{(n)} = 0,$$

where α is less than twice the minimum eigenvalue of the homogeneous equation. He has shown that this iterative scheme converges to the true solution or to the solution with the minimum norm in the case of nonuniqueness. This method can also be regarded as a regularization procedure.

EXAMPLE 9.2.5. Caldwell (1994) considers the following five equations:

- (i) $\int_0^1 e^{xs} \phi(s) ds = \frac{e^{(x+1)} - 1}{x+1}, \quad \phi(x) = e^x,$
- (ii) $\int_0^1 \sin xs \phi(s) ds = \frac{\sin x - x \cos x}{x^2}, \quad \phi(x) = x,$
- (iii) $\int_0^1 \frac{\phi(s)}{x+s+\epsilon} ds = 1 + (x+\epsilon) \ln \left(\frac{x+\epsilon}{1+x+\epsilon} \right), \quad \phi(x) = x,$
- (iv) $\int_0^1 \frac{\phi(s)}{\sqrt{x+s+\epsilon}} ds = \frac{1}{3} [\{2 - 4(x+\epsilon)\}\sqrt{1+x+\epsilon} + 4(x+\epsilon)\sqrt{x+\epsilon}], \quad \phi(x) = x,$

(v)
$$\int_0^1 \ln|x-s|\phi(s) \, ds$$
$$= \frac{1}{2} [x^2 \ln x + (1-x^2) \ln(1-x) - x - \frac{1}{2}], \quad \phi(x) = x.$$

Table 9.2.5 gives the results obtained by Caldwell. In this table the last 5 columns represent the order of error for the corresponding method and the FK1, and the ‘+’ sign indicates that the error is greater than 10^0 . It is clear from this table that, in general, the direct application of a quadrature rule does not give good results. The modified quadrature is only a little better, the regularized quadrature gives the best results, and the iteration the next best results. For the FK1 in Eq (v) all methods give acceptable results. In his computations, the maximum value of n Caldwell uses is 40. ■

Table 9.2.5.

Method	Rule	(i)	(ii)	(iii)	(iv)	(v)
Quadrature	Boundary-integral	+	+	+	+	10^{-2}
	Gauss-Legendre	+	+	+	+	10^{-2}
	Gauss-Chebyshev	+	+	+	+	10^{-2}
Regularized Quadrature	Boundary-integral	10^{-2}	10^{-3}	10^0	10^{-1}	10^{-2}
	Gauss-Legendre	10^{-4}	10^{-3}	10^0	10^{-2}	10^{-2}
	Gauss-Chebyshev	10^{-2}	10^{-2}	10^0	10^{-2}	10^{-2}
Modified Quadrature	Gauss-Legendre	+	+	+	10^0	10^{-3}
	Gauss-Chebyshev	10^{-1}	10^0	+	10^0	10^{-2}
	Midpoint rule	10^0	10^0	+	10^{-2}	10^{-3}
Iteration	Gauss-Legendre	10^{-1}	10^{-1}	10^0	10^0	10^{-2}
	Gauss-Chebyshev	10^{-1}	10^{-1}	10^0	10^0	10^{-2}
	Midpoint rule	10^{-2}	10^{-1}	10^0	10^0	10^{-3}

Other regularization methods, for example by Lavrentiev (1967) and (Tikhonov 1963), are discussed in Kythe and Puri (2002, p. 337-338).

9.3. Integral Equations of the Second Kind

We discuss numerical methods for obtaining approximate solutions of integral equations of the second kind (FK2) which are defined by Eq (9.1.2). Although quadrature rules solve an FK2 and yield its approximate solution $\tilde{\Phi} = \{\tilde{\phi}(x_0), \dots, \tilde{\phi}(x_n)\}$, these values are used in the Nyström methods, which are discussed in §9.1. Our main objective in this chapter is to present numerical methods based on quadrature that compute the approximation solution $\tilde{\Phi}(x)$.

9.3.1. Quadrature Methods. Let λ be a regular value of the kernel $k(x, s)$, and the functions $k(x, s)$ and $f(x)$ be at least piecewise continuous on $[a, b]$. To obtain an approximate solution of the integral $\int_a^b F(s) ds$, we choose a quadrature rule $Q(F) = \sum_{j=0}^n w_j F(s_j)$, where w_j are the weights and s_j the nodes taken on the interval $[a, b]$. Then we replace Eq (9.1.2) by

$$\tilde{\phi}(x) - \lambda \sum_{j=0}^n w_j k(x, s_j) \tilde{\phi}(s_j) = f(x), \quad (9.3.1)$$

where $\tilde{\phi}(x)$ denotes the approximate solution of the FK2. The solution $\tilde{\phi}(x)$ is computed by the Nyström method after setting $x = x_i$, $i = 0, 1, \dots, n$. This procedure replaces Eq (9.3.1) by

$$\tilde{\phi}(x_i) - \lambda \sum_{j=0}^n w_j k(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad i = 0, 1, \dots, n, \quad (9.3.2)$$

which in matrix notation is

$$(\mathbf{I} - \lambda \mathbf{kD}) \tilde{\Phi} = \mathbf{f}, \quad (9.3.3)$$

where $\mathbf{k} = [k(x_i, s_j)]^T$, $\mathbf{D} = \text{diag}(w_0, w_1, \dots, w_n)$, and $\mathbf{f} = [f_0, f_1, \dots, f_n]^T$. Since we have assumed that λ is a regular value of the kernel, the system (9.3.3) has a unique solution. However, for a choice of a quadrature rule the matrix $(\mathbf{I} - \lambda \mathbf{kD})$ in the system (9.3.3) may become singular. But under certain restrictions on λ , $k(x, s)$, and $f(x)$, the matrix $(\mathbf{I} - \lambda \mathbf{kD})$ will remain nonsingular provided the chosen rule $Q(F)$ yields a ‘sufficiently accurate’ quadrature. These restrictions are discussed below.

EXAMPLE 9.3.1. (Baker 1978, p. 357) Consider Eq (9.1.2) with $\lambda = 1$ and

$$k(x, s) = \begin{cases} x(1-s) & \text{if } 0 \leq x \leq s \leq 1, \\ s(1-x) & \text{if } 0 \leq s \leq x \leq 1. \end{cases}$$

Note that $\lambda \neq j^2 \pi^2$, $j = 0, 1, 2, \dots$, is a regular value of the kernel. The solution $\phi(x)$ is unique if $f(x) \in C^2[0, 1]$. We choose the trapezoidal rule T with step size $h = 1/n$:

$$T(f) = \sum_{j=0}^{n+1} {}'' h f(jh).$$

Then Eq (9.3.2) becomes

$$\tilde{\phi}(ih) - h \sum_{j=0}^{n+1} {}'' k(ih, jh) \tilde{\phi}(jh) = f(ih), \quad i = 0, 1, \dots, n.$$

The matrix $(\mathbf{I} - \mathbf{KD})$ is nonsingular since $\lambda = 1$ and $\lambda \notin \{4h^{-2} \sin^2(\pi jh/2)\}$ for $j = 1, 2, \dots, (n - 1)$, so that λ is a regular value. This yields a unique solution $\tilde{\phi} = [\tilde{\phi}(0), \tilde{\phi}(h), \dots, \tilde{\phi}(1)]^T$. It can be shown that $\tilde{\phi}(0) = f(0)$, $\tilde{\phi}(1) = f(1)$, and $h^{-2} \delta^2 \tilde{\phi}(jh) + \lambda \tilde{\phi}(jh) = h^{-2} \delta^2 f(jh)$ for $j = 1, 2, \dots, n$, where δ is the central difference operator defined by $\delta \tilde{\phi}(jh) = \tilde{\phi}((j + 1/2)h) - \tilde{\phi}((j - 1/2)h)$. Thus, $\delta^2 \tilde{\phi}(jh) = \tilde{\phi}((j + 1)h) - 2\tilde{\phi}(jh) + \tilde{\phi}((j - 1)h)$. ■

EXAMPLE 9.3.2. Consider Love’s equation

$$\phi(x) + \frac{1}{\pi} \int_{-1}^1 \frac{d}{d^2 + (x - s)^2} \phi(s) ds = f(x), \quad -1 \leq x \leq 1,$$

which occurs in electrostatics. For $d = -1$, we have $k(x, s) = -\frac{1}{\pi[1 + (x - s)^2]}$, $f(x) = 1$; using the trapezoidal rule, we get

$$\tilde{\phi}(ih - 1) - h \sum_{j=0}^{n+1} \frac{\tilde{\phi}(jh - 1)}{\pi[1 + (i - j)^2 h^2]} = 1,$$

where $h = 2/n, i = 0, 1, \dots, n$. The results are given in Table 9.3.2.

Table 9.3.2.

<i>n</i>	8	16	32	64
<i>x</i> = ±1.0	1.63639	1.63887	1.63949	1.63964
<i>x</i> = ±0.75	1.74695	1.75070	1.75164	1.75188
<i>x</i> = ±0.5	1.83641	1.84089	1.84201	1.84229
<i>x</i> = ±0.25	1.89332	1.89804	1.89922	1.89952
<i>x</i> = 0.0	1.91268	1.91744	1.91863	1.91893

For computational details, see [quadrature.nb](#) on the CD-R. Baker (1978, p.358) uses the Romberg scheme to obtain the following results, where the underlines indicate similar values:

	9 points	17 points	33 points	65 points
<i>x</i> = ±1.0	1.63673	1.63969	<u>1.63970</u>	<u>1.63970</u>
<i>x</i> = ±0.75	1.75183	1.75196	<u>1.75195</u>	<u>1.75195</u>
<i>x</i> = ±0.5	1.84215	1.84239	<u>1.84238</u>	<u>1.84238</u>
<i>x</i> = ±0.25	1.89969	<u>1.89961</u>	<u>1.89961</u>	<u>1.89961</u>
<i>x</i> = 0.0	1.91934	<u>1.91903</u>	<u>1.91903</u>	<u>1.91903</u> ■

RESTRICTIONS. (i) If the kernel is degenerate, e.g., if

$$k^{[m]}(x, s) = \sum_{m=0}^N X_m(x) S_m(s),$$

then the exact solution of Eq (9.1.2) is of the form

$$\phi(x) = f(x) + \lambda \sum_{m=0}^N a_m X_m(x),$$

where $(\mathbf{I} - \lambda \mathbf{A}) \mathbf{a} = \mathbf{b}$, with

$$A_{ij} = \int_a^b X_j(x) S_i(x) dx, \quad b_i = \int_a^b f(x) S_i(x) dx.$$

Similarly, the solution of Eq (9.3.1) is of the form

$$\tilde{\phi}(x) = f(x) + \lambda \sum_{m=0}^N \tilde{a}_m X_m(x),$$

where $(\mathbf{I} - \lambda \tilde{\mathbf{A}}) \tilde{\mathbf{a}} = \tilde{\mathbf{b}}$, with

$$\tilde{A}_{ij} = \sum_{m=0}^N w_m X_j(s_m) S_i(s_m), \quad \tilde{b}_i = \sum_{m=0}^N w_m f(s_m) S_i(s_m).$$

To keep the quantities $\|\mathbf{A} - \tilde{\mathbf{A}}\|$ and $\|\mathbf{b} - \tilde{\mathbf{b}}\|$ small, we must choose the quadrature rule $Q(F)$ according to the behavior of both $k(x, s)$ and $f(x)$. But if the system $(\mathbf{I} - \lambda \mathbf{A}) \mathbf{a} = \mathbf{b}$ becomes ill conditioned, it may not be possible to compute \mathbf{a} . This may happen for certain choices of λ and $k(x, s)$ which in turn impart ill-conditioning to the whole problem. If this is the case, we will not be able to compute $\tilde{\phi}(x)$.

(ii) If the kernel $k(x, s)$ or the function $f(x)$ is known or suspected to be badly behaved, we can use the *method of deferred correction* (see §9.3.5(a)). With this approach the accuracy of the initial approximation $\tilde{\phi}(x)$ does not remain important. As a rule, we choose a quadrature rule for which we can ‘predict’ the truncation error

$$t(x) = \phi(x) - \lambda \sum_{j=0}^n w_j k(x, s_j) \phi(s_j) - f(x).$$

This means that if we want to find an accurate initial solution $\tilde{\phi}$, we should choose a quadrature rule such that $\|t\|_{\infty} = \sup_{0 \leq i \leq n} |t(s_i)|$ is small. Whether this condition is satisfied depends on the properties of the quadrature rule as well as on the properties of the differentiability of $\phi(x)$. Since

$$\phi(x) = f(x) + \lambda \int_a^b k_{\lambda}(x, s) f(s) ds,$$

where $k_\lambda(x, s)$ is the resolvent kernel, any bad behavior of $f(x)$ shall influence the solution $\phi(x)$.

9.3.2. Modified Quadrature Methods. A quadrature method is modified in the case when $k(x, s)$ is badly behaved at $x = s$ by using the following method to reduce the error: Write Eq (9.1.2) as

$$\phi(x) - \lambda \phi(x) \int_a^b k(x, s) ds - \lambda \int_a^b k(x, s) [\phi(s) - \phi(x)] ds = f(x), \quad (9.3.4)$$

and use a quadrature rule $Q(F)$ to get

$$\hat{\phi}(x) [1 - \lambda A(x)] - \lambda \sum_{j=0}^n w_j k(x, s_j) [\hat{\phi}(s_j) - \hat{\phi}(x)] = f(x), \quad (9.3.5)$$

where $A(x) = \int_a^b k(x, s) ds$. Hence,

$$\hat{\phi}(x) [1 - \lambda \Delta(x)] - \lambda \sum_{j=0}^n w_j k(x, s_j) \hat{\phi}(s_j) = f(x), \quad (9.3.6)$$

where

$$\Delta(x) = A(x) - \sum_{j=0}^n w_j k(x, s_j). \quad (9.3.7)$$

If we set $x = x_i, i = 0, 1, \dots, n$ in (9.3.7), we obtain by the Nyström method

$$\hat{\phi}(x_i) [1 - \lambda \Delta(x_i)] - \lambda \sum_{j=0}^n w_j k(x_i, s_j) \hat{\phi}(s_j) = f(x_i),$$

which in matrix notation becomes

$$(\mathbf{I} - \lambda (\Delta - \mathbf{kD})) \tilde{\Phi} = \mathbf{f},$$

where \mathbf{I} is the identity matrix, $\mathbf{k} = (k(x_i, s_j))_{ij}$, $\Delta = \text{diag}\{\Delta(x_0), \Delta(x_1), \dots, \Delta(x_n)\}$, and $\mathbf{D} = \text{diag}\{w_0, w_1, \dots, w_n\}$. It is important to compute $A(x)$ accurately. This modified quadrature method is useful when $k(x, s)$ is discontinuous at $x = s$ and also when $k(x, s)$ is weakly singular (see §9.5). It is found that $\hat{\phi}$ gives better approximations than ϕ in the above cases.

EXAMPLE 9.3.3. Consider Love's equation (see [Example 9.3.2](#)). Here

$$A(x) = \int_{-1}^1 k(x, s) ds = -\frac{1}{\pi} \tan^{-1} \left(\frac{2}{x^2} \right).$$

Use the trapezoidal rule with $h = 2/n$. The values of $\hat{\phi}$ at $x = (-1)(0.25)1$ are presented in Table 9.3.3.

Table 9.3.3.

	$n = 8$	$n = 16$	$n = 32$	$n = 64$
$x = \pm 1.0$	1.63838	1.63937	1.63961	1.63967
$x = \pm 0.75$	1.751071	1.75164	1.75188	1.75194
$x = \pm 0.5$	1.84135	1.84213	1.84232	1.84237
$x = \pm 0.25$	1.89874	1.89940	1.89956	1.89960
$x = 0.0$	1.91821	1.91883	1.91898	1.91902 ■

Another modification is possible in the case when $k(x, s) = g(s) \kappa(x, s)$ in (9.1.2), where $g(s)$ is badly behaved; e.g., $g(s) = \sqrt{s}$ so that $g'(0)$ is unbounded. Then we use a quadrature rule for products (see §9.3.6), i.e.,

$$\int_a^b g(s) p(s) ds = \sum_{j=0}^n v_j p(s_j). \quad (9.3.8)$$

While a quadrature rule produces a system of the form (9.3.2), the product rule (9.3.8) yields a system of the form

$$\tilde{\phi}(x_i) - \lambda \sum_{j=0}^n v_j \kappa(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad i = 0, 1, \dots, n.$$

If $g(x) > 0$, then it is possible to develop a Gaussian quadrature to approximate the integral (9.3.8). However, this modified method is successful if the functions $f(x)$ and $\kappa(x, s)$ are smooth. Otherwise the product integration method discussed in §9.3.6 is better to use.

9.3.3. Quadrature Formulas. If we replace the integral in Eq (9.1.2) by a quadrature formula of the form (2.6.1) where $w_j \geq 0$ and $\sum_{j=1}^n w_j = b - a$, then Eq (9.1.2) becomes

$$\phi(x) - \lambda \sum_{j=1}^n w_j k(x, x_j) \phi(x_j) = f(x) + \lambda \varepsilon(x). \quad (9.3.9)$$

If we set $x = x_i$, $i = 1, 2, \dots, n$, and neglect $\varepsilon(x) = \varepsilon(x_j)$, we obtain the system of algebraic equations for the unknown approximate values of $\tilde{\phi}(x_i)$ as

$$\tilde{\phi}(x_i) - \lambda \sum_{j=1}^n w_j k(x_i, x_j) \tilde{\phi}(x_j) = f(x_i), \quad i = 1, 2, \dots, n, \quad (9.3.10)$$

or

$$\begin{aligned}
 & \tilde{\phi}(x_1) [1 - \lambda w_1 k(x_1, x_1)] - \lambda \tilde{\phi}(x_2) w_2 k(x_1, x_2) - \cdots \\
 & \quad - \lambda \tilde{\phi}(x_n) w_n k(x_1, x_n) = f(x_1), \\
 & -\lambda \tilde{\phi}(x_1) w_1 k(x_2, x_1) + \tilde{\phi}(x_2) [1 - \lambda w_2 k(x_2, x_2)] - \cdots \\
 & \quad - \lambda \tilde{\phi}(x_n) w_n k(x_2, x_n) = f(x_2), \\
 & \quad \vdots \\
 & -\lambda \tilde{\phi}(x_1) w_1 k(x_n, x_1) - \lambda \tilde{\phi}(x_2) w_2 k(x_n, x_2) - \cdots \\
 & \quad + \tilde{\phi}(x_n) [1 - \lambda w_n k(x_n, x_n)] = f(x_n).
 \end{aligned} \tag{9.3.11}$$

Solve this system and substitute the values of $\tilde{\phi}(x_1), \dots, \tilde{\phi}(x_n)$ into Eq (9.3.9). This will yield the required approximate solution of Eq (9.1.2). Any quadrature formulas can be used for this method.

EXAMPLE 9.3.4. (Mikhlin and Smolitskiy 1967, p.286) The plane interior Dirichlet problem for the region lying inside a sufficiently small contour C is governed by the equation

$$\phi(t) - \frac{1}{\pi} \int_C \frac{\cos(\nu, r)}{r} \phi(\tau) d\sigma = f(t), \tag{9.3.12}$$

where t and τ are the parameters that determine the position of points on the contour C ; r the distance between points corresponding to values of these parameters; ν the exterior normal to C at τ ; $d\sigma$ the arc length element; $\phi(t)$ the unknown function; and $f(t)$ the prescribed function. Eq (9.3.12) is obtained if a harmonic function is sought in the form of a potential of a double layer with density $\phi(\tau)$ (see [Kythe 1996](#), p.21). Let C be defined as the ellipse $x = a \cos t$, $y = b \sin t$, $a = 5$, $b = 3$, and let $f(t) = x^2 + y^2 = 25 - 16 \sin^2 t$. Then

$$\begin{aligned}
 \int_C \frac{\cos(\nu, r)}{r} \phi(\tau) d\sigma &= -\frac{b}{2a} \int_{-\pi}^{\pi} \frac{\phi(\tau)}{1 - e^2 \cos^2 \frac{t+\tau}{2}} d\tau \\
 &= -\frac{3}{10\pi} \int_{-\pi}^{\pi} \frac{\phi(\tau)}{0.68 - 0.32 \cos(t+\tau)} d\tau,
 \end{aligned}$$

where $e = 4/5$ is the eccentricity of the ellipse. Thus, Eq (9.3.12) reduces to

$$\phi(\tau) + \frac{3}{10\pi} \int_{-\pi}^{\pi} \frac{\phi(\tau)}{0.68 - 0.32 \cos(t+\tau)} d\tau = 25 - 16 \sin^2 t.$$

Note that the unknown function $\phi(t)$ is periodic of period π , i.e., $\phi(-t) = \phi(\pi - t) = \phi(t)$. For quadrature we shall use the trapezoidal rule with 12 intervals of equal length $\pi/6$ from $-\pi$ to π (see [Fig. 9.3.1](#) on page 545).

Because of the periodic nature of $\phi(t)$, we adopt the notation: $\phi(0) = y_1$, $\phi(\pi/6) = y_2$, $\phi(\pi/3) = y_3$, $\phi(\pi/2) = y_4$. This leads to a system of four equations:

$$\begin{aligned} 1.18889 y_1 + 0.352697 y_2 + 0.311355 y_3 + 0.147059 y_4 &= 25, \\ 0.176349 y_1 + 1.34457 y_2 + 0.323407 y_3 + 0.153678 y_4 &= 21, \\ 0.155678 y_1 + 0.323407 y_2 + 1.34457 y_3 + 0.176349 y_4 &= 13, \\ 0.147059 y_1 + 0.311355 y_2 + 0.352697 y_3 + 1.18889 y_4 &= 9, \end{aligned}$$

which yields

$$y_1 = 16.0294, \quad y_2 = 12.2647, \quad y_3 = 14.7353, \quad y_4 = 0.970595. \tag{9.3.13}$$

The function $\phi(t)$ can now be constructed by expanding it as a Fourier cosine series which in view of its periodicity can be written as $\phi(t) = \sum_{n=0}^\infty a_n \cos 2nt$. Taking the first four terms of this series and using the values of y_1, y_2, y_3, y_4 from (9.3.13), we find that

$$\begin{aligned} a_0 + a_1 + a_2 + a_3 &= y_1, \\ a_0 + \frac{a_1}{2} - \frac{a_1}{2} - a_3 &= y_2, \\ a_0 - \frac{a_1}{2} - \frac{a_1}{2} + a_3 &= y_3, \\ a_0 - a_1 + a_2 - a_3 &= y_4, \end{aligned}$$

which, with the above values of y_1, \dots, y_4 , yield $a_0 = 8.5, a_1 = 7.5294, a_2 = 0, a_3 = 1.18424 \times 10^{-15}$. Ignoring the value of a_3 , which is very small, we obtain $\phi(t) \approx 8.5 + 7.5294 \cos 2t$. This matches with the exact solution (see [Mikhlin and Smolitskiy 1967](#), p.287)

$$\phi(t) = \frac{17}{2} + \frac{128}{17} \cos 2t = 8.5 + 7.5294117 \cos 2t.$$

For computational details with the trapezoidal rule, see [dirichlet1.nb](#) on the CD-R. The results obtained from using other quadrature rules are presented in Table 9.3.4.

Table 9.3.4.

Rule	a_0	a_1	a_2	a_3
Exact solution	8.5	7.5294117	0.0	0.0
Trapezoidal ($n = 12$)	8.5	7.529	0.0	1.18424(−15)
Rectangular ($n = 12$)	8.5	7.5294	0.0	1.18424(−15)
Simpson’s ($n = 12$)	8.29185	8.68164	−1.23377	0.62602
Gauss-Legendre ($n = 12$)	8.573	7.10315	−0.001688	−0.0662033
Weddle ($n = 12$)	8.50009	7.48573	0.0108996	0.0021237

Note that the Gauss-Legendre formula shows poor results simply because we have approximated the values of $\phi(t)$ in the integrand by those of $\phi(t_i)$ (which are y_1, y_2, y_3 , and y_4 , respectively). For computational details, see [dirichlet2.nb](#) and [dirichlet3.nb](#) on the CD-R. ■

9.3.4. Error Analysis. Instead of the system (9.3.10), we consider the corresponding homogeneous system (with $f(x_i) = 0, i = 1, 2, \dots, n$). The determinant of this system is

$$D(\lambda) = \begin{vmatrix} 1 - \lambda w_1 k(x_1, x_1) & -\lambda w_2 k(x_1, x_2) & \dots & -\lambda w_n k(x_1, x_n) \\ -\lambda w_1 k(x_2, x_1) & 1 - \lambda w_2 k(x_2, x_2) & \dots & -\lambda w_n k(x_2, x_n) \\ \dots & \dots & \dots & \dots \\ -\lambda w_1 k(x_n, x_1) & -\lambda w_2 k(x_n, x_2) & \dots & 1 - \lambda w_n k(x_n, x_n) \end{vmatrix}. \quad (9.3.14)$$

We solve the equation $D(\lambda) = 0$ and determine those values of λ for which the system (9.3.14) has a solution $\tilde{\phi}(x_i) \neq 0$. Note that these values of λ approximate eigenvalues, which can be used to find approximate eigenfunctions from (9.3.14).

To find the error, let D_{ij} denote the cofactor of the element in the i -th row and j -th column in the determinant (9.3.14). Then the approximate solution of the system (9.3.10) is given by

$$\tilde{\phi}(x_i) = \frac{\sum_{j=1}^n D_{ij} f(x_j)}{D(\lambda)}, \quad i = 1, 2, \dots, n.$$

We shall estimate how much these approximate values $\tilde{\phi}(x_i)$ differ from the exact values $\phi(x_i), i = 1, \dots, n$. Assuming that the functions $k(x, s)$ and $f(x)$ have a certain finite number p of continuous derivatives, i.e., $k \in C^p(a, b)$ and $f \in C^p(a, b)$, the function ϕ shall also belong to the class $C^p(a, b)$. Let

$$\begin{aligned} H^{(0)} &= \text{ub}_{a \leq x \leq b} |\phi(x)|, & H^{(q)} &= \text{ub}_{a \leq x \leq b} |\phi^{(q)}(x)|, \\ N^{(0)} &= \text{ub}_{a \leq x \leq b} |f(x)|, & N^{(q)} &= \text{ub}_{a \leq x \leq b} |f^{(q)}(x)|, \\ M_x^{(q)} &= \text{ub}_{a \leq s \leq x \leq b} \left| \frac{d^q}{dx^q} k(x, s) \right|, & M_y^{(q)} &= \text{ub}_{a \leq s \leq x \leq b} \left| \frac{d^q}{ds^q} k(x, s) \right|, \\ M^{(0)} &= \text{ub}_{a \leq s \leq x \leq b} |k(x, s)|, & q &= 1, 2, \dots, p. \end{aligned}$$

Then, by using Leibniz' rule (1.1.5), the derivatives of the integrand in Eq (9.1.2) are evaluated as

$$\begin{aligned} \left| \frac{d^q}{dx^q} [k(x, s)\phi(s)] \right| &\leq H^{(0)} M_s^{(q)} c_q^1 H^{(1)} M_s^{(q-1)} + \dots + c_q^{(q-1)} H^{(q-1)} M_s^{(1)} \\ &+ H^{(q)} M^{(0)} \equiv T^{(q)} \quad (\text{say}). \end{aligned} \quad (9.3.15)$$

If E denotes the maximum modulus of the error $\varepsilon(x)$ in (9.3.9) when we replace the integral $\int_a^b k(x, s)\phi(s) ds$ by the sum, i.e., when we take

$$\int_a^b k(x, s)\phi(s) ds - \sum_{j=1}^n w_j k(x, x_j) \phi(x_j) = \varepsilon(x),$$

so that $|\varepsilon(x)| \leq E$ and $|\varepsilon_j| = |\varepsilon(x_j)| \leq E$, then E can be easily evaluated from (9.3.15) in the form $E \leq d_n T^{(q)}$, where d_n is a factor of the formula; thus, for example, for the trapezoidal rule:

$$E \leq \frac{(b-a)^3}{12(n-1)^2} T^{(2)}; \quad (9.3.16a)$$

and for the Gauss-Legendre rule:

$$E \leq \frac{(b-a)^{2n+1}}{2n+1} \left[\frac{1 \cdot 2 \cdot 3 \cdots n}{(n+1) \cdots (2n)} \right]^2 \frac{T^{(2n)}}{1 \cdot 2 \cdot 3 \cdots (2n)}. \quad (9.3.16b)$$

We finally obtain the formula

$$\begin{aligned} T^{(q)} &= H^{(0)} M_s^{(q)} + c_q^1 H^{(1)} M_s^{(q-1)} + \cdots + H^{(q)} M^{(0)} \\ &\leq N^{(0)} M_s^{(q)} + c_q^1 N^{(1)} M_s^{(q-1)} + \cdots + N^{(q)} M^{(0)} \\ &\quad + |\lambda| (b-a) \left[M^{(0)} M_s^{(q)} + c_q^1 M_x^{(1)} M_s^{(q-1)} + \cdots + M_x^{(q)} M^{(0)} \right] H^{(0)} \\ &\equiv P_q + Q_q H^{(0)}, \end{aligned}$$

where P_q and Q_q are known. As noted above, the estimate of the error E is then of the form

$$E \leq d_n T^{(q)} \leq d_n (P_q + Q_q H^{(0)}).$$

EXAMPLE 9.3.5. (Kantorovich and Krylov 1958, pp.108–111) Consider the equation

$$\phi(x) - \frac{1}{2} \int_0^1 e^{xs} \phi(s) ds = 1 - \frac{e^x - 1}{2x}. \quad (9.3.17)$$

We use the Gauss-Legendre quadrature for the interval $(0, 1)$. The system (9.3.11) with $n = 2$ is

$$\begin{aligned} [1 - \lambda w_1 k(x_1, x_1)] \tilde{\phi}(x_1) - \lambda w_2 k(x_1, x_2) \tilde{\phi}(x_2) &= f(x_1), \\ -\lambda w_1 k(x_1, x_1) \tilde{\phi}(x_1) + [1 - \lambda w_2 k(x_2, x_2)] \tilde{\phi}(x_2) &= f(x_2). \end{aligned}$$

Note that $\lambda = 0.5$, $w_1 = w_2 = 0.5$, and $x_1 = 0.2113248654$, $x_2 = 0.7886751346$ (see Abramowitz and Stegun 1968, p.921). Then the determinant of this system is

$$D(\lambda) = \begin{vmatrix} 0.738582 & -0.29534 \\ -0.29534 & 0.544334 \end{vmatrix} = 0.307424.$$

The determinants D_1 and D_2 are

$$D_1 = \begin{vmatrix} 0.443242 & -0.29534 \\ 0.238927 & 0.544334 \end{vmatrix} = 0.307404,$$

$$D_2 = \begin{vmatrix} 0.738582 & 0.443242 \\ -0.29534 & 0.238927 \end{vmatrix} = 0.307374.$$

Thus, $\tilde{\phi}(x_1) = D_1/D(\lambda) = 0.999935$, $\tilde{\phi}(x_2) = D_2/D(\lambda) = 0.999839$, and the approximate solution of Eq (9.3.17) is

$$\tilde{\phi}(x) = 1 + 0.25 \left[0.999935 e^{x_1 x} + 0.999839 e^{x_2 x} \right] - \frac{e^x - 1}{2x}.$$

The exact solution is $\phi(x) = 1$. Comparing these solutions at the points $0, x_1, x_2$, and 1 , we find that the difference $|\phi(x) - \tilde{\phi}(x)|$ is 0.000056 , 0.000065 , 0.000161 and 0.000301 , respectively, which imply that the errors are of the order $O(10^{-3})$.

We now compute a precise estimate of the error E . The quantity B has the bound $(0.738582 + 0.29534)/2 = 3.36318$; so we may take $B = 3.4$. The free term $f(x)$ and its derivatives, expanded in series, are

$$\begin{aligned} f(x) &= \frac{1}{2} - \frac{x}{4} - \frac{x^2}{12} - \frac{x^3}{48} - \frac{x^4}{240} - \frac{x^5}{1440} - \frac{x^6}{10080} - \cdots, \\ f'(x) &= -\left(\frac{1}{4} + \frac{x}{6} + \frac{x^2}{16} + \frac{x^3}{60} + \frac{x^4}{288} + \frac{x^5}{1680} + \cdots\right), \\ f''(x) &= -\left(\frac{1}{6} + \frac{x}{8} + \frac{x^2}{20} + \frac{x^3}{72} + \frac{x^4}{336} + \cdots\right), \\ f'''(x) &= -\left(\frac{1}{8} + \frac{x}{10} + \frac{x^2}{24} + \frac{x^3}{84} + \cdots\right), \\ f^{(4)}(x) &= -\left(\frac{1}{10} + \frac{x}{12} + \frac{x^2}{28} + \cdots\right). \end{aligned}$$

Then, considering the bounds for $f, f', f'', f''', f^{(4)}$ in the interval $(0, 1)$, we may take

$$N^{(0)} = 0.5 = N^{(1)}, \quad N^{(2)} = 0.36, \quad N^{(3)} = 0.28, \quad N^{(4)} = 0.22.$$

The kernel and its derivatives are

$$k(x, s) = e^{xs}, \quad k_x^{(i)} = s^i e^{xs}, \quad k_s^{(i)} = x^i e^{xs}, \quad i = 1, 2, 3, 4.$$

Then for their bounds in the interval $(0, 1)$ we may take

$$M^{(0)} = M_x^{(1)} = \cdots = M_x^{(4)} = M_s^{(1)} = \cdots = M_s^{(4)} = e.$$

Hence,

$$\begin{aligned} P_4 &= N^{(0)} M_s^{(4)} + c_4^1 N^{(1)} M_s^{(3)} + c_4^2 N^{(2)} M_s^{(2)} + c_4^3 N^{(3)} M_s^{(1)} \\ &\quad + N^{(4)} M^{(0)} < 8e < 22, \\ Q_4 &= |\lambda| (b-a) \left[M^{(0)} M_s^{(4)} + c_4^1 M_x^{(1)} M_s^{(3)} + c_4^2 M_x^{(2)} M_s^{(2)} \right. \\ &\quad \left. + c_4^3 M_x^{(3)} M_s^{(1)} + M_x^{(4)} M^{(0)} \right] = 8e^2 < 60. \end{aligned}$$

Then $T^{(4)} = P_4 + Q_4 H^{(0)}$, where $H^{(0)}$ denotes the upper bound of $\phi(s)$ on the interval $[0, 1]$. Next, from (9.3.16b)

$$E = d_2 T^{(4)} = \frac{1}{5} \left[\frac{1 \cdot 2}{3 \cdot 4} \right]^2 \frac{T^{(4)}}{1 \cdot 2 \cdot 3 \cdot 4} = \frac{1}{4320} T^{(4)};$$

thus, $d_2 = \frac{1}{4320}$. From (9.3.17) we compute the upper bound S of $|\tilde{\phi}(x)|$ as

$$\begin{aligned} S &= 0.25 (e^{x_1} + e^{x_2}) + \lim_{x \rightarrow 0} \left(1 - \frac{e^x - 1}{2x} \right) \\ &= 0.85936 + 0.5 = 1.35936, \end{aligned}$$

so we may take $S = 1.4$, and obtain

$$H^{(0)} \leq \frac{1.4 + [e(3.4)(1)(0.5) + 1] \cdot (0.5)(1/4320)(22)}{1 - [e(3.4)(1)(0.5) + 1] \cdot (0.5)(1/4320)(60)} = 1.47176.$$

Hence, we get the difference

$$\begin{aligned} |\phi(x) - \tilde{\phi}(x)| &= |\lambda| [1 + |\lambda| B M^{(0)}(b-a)] d_2 (P_4 + Q_4 H^{(0)}) \\ &= 0.5 [1 + (0.5)(3.4)(e)(1)] \frac{1}{4320} (22 + (60)(1.46911)) = 0.07166. \end{aligned}$$

Thus, as we have seen earlier, the error is really of the order 10^{-3} , which is considerably lower than the above estimate of .07166. The above estimate, although lengthy, has definitely established that $\lambda = 1/2$ is not an eigenvalue of Eq (9.3.17), and, therefore, this equation has a unique solution. For computational details, see [error1.nb](#) on the CD-R.

If we take $n = 4$, we find that $D(\lambda) = 0.305786$, and $D_1 = D_2 = D_3 = D_4 = 0.30586$, thus, $\tilde{\phi}_1 = \tilde{\phi}_2 = \tilde{\phi}_3 = \tilde{\phi}_4 = 1$. The approximate solution is

$$\begin{aligned} \tilde{\phi}(x) &= 1 + 0.25 \left[e^{0.0694318442x} + e^{0.3300094782x} + e^{0.669905218x} \right. \\ &\quad \left. + e^{0.9305681556x} \right] - \frac{e^x - 1}{2x}. \end{aligned}$$

The error at $x = 0, 1$ is the same as for $n = 2$, viz., 0.000056 and 0.000301, respectively. The rest of the analysis also matches that of the case $n = 2$. Similarly, for $n = 8$ we get $D(\lambda) = 0.305786$, and the remaining data are the same as in case the case $n = 4$. For computational details for $n = 4$ and 8, see [error2.nb](#) and [error3.nb](#) on the CD-R. ■

9.3.5. Expansion Methods. An expansion method for an FK2 of the form (9.1.2) determines the approximate solution $\tilde{\phi}(x)$ as a linear combination of the form $\sum_{j=0}^n a_j p_j(x)$ of prescribed functions $p_j(x)$, $j = 0, 1, \dots, n$, which are generally taken as one of the orthogonal polynomials. We use one of the quadrature rules to obtain the approximate solution $\tilde{\phi}$ as a linear combination of the form

$$\tilde{\phi}(x) = \sum_{j=0}^n a_j k(x, s_j) + f(x), \quad \text{where} \quad a_j = \lambda w_j \tilde{\phi}(s_j).$$

For example, we can use the Chebyshev polynomials $T_j(x)$ of the first kind and match them with the vector $[\tilde{\phi}(s_0), \tilde{\phi}(s_1), \dots, \tilde{\phi}(s_n)]^T$, where the nodes s_j and the polynomials $T_j(x)$, $j = 0, 1, \dots, n$, match with each other. If we employ the Clenshaw-Curtis quadrature rule (see §3.3.1), we have $s_j = \cos(j\pi/n)$, and this leads to the approximation

$$\tilde{\phi}(x) = \sum_{m=0}^n \tilde{a}_m T_m(x), \quad (9.3.18)$$

where

$$\tilde{a}_m = \frac{2}{n} \sum_{i=1}^{n+1} \tilde{\phi}\left(\cos \frac{j\pi}{n}\right) T_m\left(\cos \frac{j\pi}{n}\right), \quad m = 0, 1, \dots, n. \quad (9.3.19)$$

EXAMPLE 9.3.6. Consider the FK2 (Young 1954a,b, El-gendi 1969)

$$\phi(x) + \frac{1}{\pi} \int_{-1}^1 \frac{\phi(s)}{1 + (x-s)^2} ds = 1, \quad -1 \leq x \leq 1.$$

For $n = 8$ El-gendi (1969) obtained

$$\begin{aligned} \tilde{a}_0 &= 1.415185, & \tilde{a}_2 &= 0.049385, & \tilde{a}_4 &= -0.001048, \\ \tilde{a}_6 &= -0.000231, & \tilde{a}_8 &= 0.0000195, & \tilde{a}_1 &= \tilde{a}_3 = \tilde{a}_5 = \tilde{a}_7 = 0. \end{aligned}$$

This suggests that the solution is symmetric about s -axis, and we can take odd coefficients $\tilde{a}_{2m+1} = 0$. Thus, we can solve only $[n/2]$ equations in the $[n/2]$ unknowns \tilde{a}_{2m} , and obtain the solution $\tilde{\phi}$ at different equally spaced $(n+1)$ values of x in the interval $[-1, 1]$. For example, if we take $n = 10$, we solve only 5 equations in 5

unknowns \tilde{a}_{2m} , $m = 0, 1, 2, 3, 4$, and get the solution at 11 equally spaced points in $[-1, 1]$, as given in Table 9.3.6. ■

Table 9.3.6.

x	0	± 0.2	± 0.4	± 0.6	± 0.8	± 1
$\tilde{\phi}(x)$	0.65740	0.66151	0.67390	0.69448	0.72248	0.75570

9.3.5(a) Deferred Correction Method. We use either Romberg's or Gregory's scheme to obtain the approximate solution $\tilde{\phi}(x)$ of the FK2 (9.1.2). We first discuss the Romberg scheme (see §2.7). Suppose we have applied the trapezoidal rule with step size $h = (b - a)/n$ to obtain the approximate solution $\tilde{\phi}(x) \equiv \tilde{\phi}_h(x)$ by solving the system

$$\tilde{\phi}_h(a + ih) - \lambda h \sum_{j=0}^{n+1} w_j k(a + ih, a + jh) \tilde{\phi}_h(a + jh) = f(a + ih), \quad (9.3.20)$$

for $i = 0, 1, \dots, n$ and for $h \in \{h_0, h_0/2, h_0/4\}$, say. Now, if we compute the vectors $\tilde{\Phi}_h$ for $h = h_0, h_0/2, h_0/4$, we obtain

3 estimates of each value of $\phi(a), \phi(a + h_0), \phi(a + 2h_0), \dots, \phi(b)$,

2 estimates of each value of $\phi(a + h_0/2), \phi(a + 3h_0/2), \dots, \phi(b - h_0/2)$, and

1 estimate of each value of $\phi(a + h_0/4), \phi(a + 3h_0/4), \dots, \phi(b - h_0/4)$.

Suppose that

$$\tilde{\phi}_h(a + ih) = \phi(a + ih) + \sum_{m=1}^N h^{2m} p_m(a + ih) + O(h^{2N+1}), \quad (9.3.21)$$

where the basis functions $p_m(x)$, $m = 1, 2, \dots, N$, are independent of h . Then, combining the estimates of the values of $\phi(a_i h_0)$ and using the deferred corrections that are similar to those of Romberg's scheme (as in Baker 1978, p.362ff.), we get

$$\begin{aligned} \tilde{\phi}_{h_0}^{[1]}(a + ih_0) &= \frac{4\tilde{\phi}_{h_0/2}(a + ih_0) - \tilde{\phi}_{h_0}(a + ih_0)}{3}, \\ \tilde{\phi}_{h_0}^{[2]}(a + ih_0) &= \frac{16\tilde{\phi}_{h_0/2}^{[1]}(a + ih_0) - \tilde{\phi}_{h_0}^{[1]}(a + ih_0)}{15}, \end{aligned}$$

and so on. This gives

$$\begin{aligned} \phi(a + ih_0) - \tilde{\phi}(a + ih_0) &= O(h_0^2), \\ \phi(a + ih_0) - \tilde{\phi}^{[1]}(a + ih_0) &= O(h_0^4), \\ \phi(a + ih_0) - \tilde{\phi}^{[2]}(a + ih_0) &= O(h_0^6), \end{aligned}$$

where the order terms are uniform in i as h_0 decreases.

If the integrand $k(x, s)\phi(s)$ in the FK2 is sufficiently differentiable with respect to s , a deferred correction method can be used to obtain the approximate solution $\tilde{\phi}$ by using *Gregory's scheme*. Suppose that an initial approximation $\tilde{\phi}(x) = \tilde{\phi}^{(0)}(x)$ is found after using a quadrature rule, say a repeated trapezoidal rule with step size $h = (b - a)/n$. Then we should compute only the vector $\tilde{\Phi}^{(0)} = [\tilde{\phi}^{(0)}(a), \tilde{\phi}^{(0)}(a + h), \dots, \tilde{\phi}^{(0)}(b)]^T$, where

$$\tilde{\phi}_h^{(0)}(a + ih) - \lambda h \sum_{j=0}^n {}'' k(a + ih, a + jh) \tilde{\phi}_h^{(0)}(a + jh) = f(a + ih), \quad (9.3.22)$$

for $i = 0, 1, \dots, n$ (compare this with (9.3.20)). If we use Gregory's scheme instead of the repeated trapezoidal rule, we get

$$\tilde{\phi}_h(a + ih) - \lambda \left\{ h \sum_{j=0}^n {}'' k(a + ih, a + jh) \tilde{\phi}_h(a + jh) + \delta_i(\tilde{\phi}) \right\} = f(a + ih), \quad (9.3.23)$$

for $i = 0, 1, \dots, n$, where $\delta_i(\tilde{\phi})$ is Gregory's correction term to the trapezoidal rule, defined by

$$\begin{aligned} \delta_i(\tilde{\phi}) &= h \sum_{m=1}^p c_m^* \left\{ \nabla^m \vartheta_i(\tilde{\phi}; b) + (-1)^m \Delta^m \vartheta_i(\tilde{\phi}; a) \right\}, \quad p \leq n, \\ \nabla^m \vartheta_i(\tilde{\phi}; b) &= \Delta^m \vartheta_i(x) \Big|_{x=b}, \\ \Delta^m \vartheta_i(\tilde{\phi}; a) &= \Delta^m \vartheta_i(x) \Big|_{x=a}, \\ \vartheta_i(x) &= \vartheta_i(\tilde{\phi}; x) = k(a + ih, x) \tilde{\phi}(x). \end{aligned} \quad (9.3.24)$$

This scheme uses the forward and backward differences Δ^m and ∇^m , respectively, defined for $m \geq 1$ by

$$\begin{aligned} \Delta^m \vartheta(x) &= \Delta^{m-1} \vartheta(x + h) - \Delta^{m-1} \vartheta(x), \\ \nabla^m \vartheta(x) &= \Delta^m \vartheta(x - mh), \end{aligned}$$

such that

$$\Delta^m \vartheta(x) = \nabla^m \vartheta(x + mh) = \sum_{j=0}^m (-1)^{j+m} \binom{m}{j} \vartheta(x + jh),$$

where $\binom{m}{j}$ denote the binomial coefficients, and the coefficients c_m^* in (9.3.24) are computed recursively by the recursive formula

$$\begin{aligned} c_0^* &= 1, \\ c_m^* &= - \left[\frac{1}{2} c_{m-1}^* + \dots + \frac{1}{m+1} c_0^* \right], \quad m = 1, 2, \dots \end{aligned}$$

(see [Henrici 1964](#), p.252), which gives their values as

$$c_1^* = \frac{1}{2}, \quad c_2^* = -\frac{1}{12}, \quad c_3^* = -\frac{1}{24}, \quad c_4^* = -\frac{19}{720}, \quad c_5^* = -\frac{3}{160}, \quad c_6^* = -\frac{863}{160480},$$

and so on. Thus, we can write the trapezoidal rule with Gregory's correction as

$$\begin{aligned} \int_a^b F(x) ds \approx & \frac{h}{2} \left[F(a) + 2F(a+h) + 2F(a+2h) + \dots + 2F(b-h) \right. \\ & \left. + F(b) \right] - \frac{h}{12} (\nabla F(b) - \Delta F(a)) - \frac{h}{24} (\nabla^2 F(b) - \Delta^2 F(a)) \\ & - \frac{19h}{720} (\nabla^3 F(b) - \Delta^3 F(a)) - \frac{3h}{160} (\nabla^4 F(b) - \Delta^4 F(a)) \\ & - \frac{863h}{60480} (\nabla^5 F(b) - \Delta^5 F(a)), \end{aligned}$$

where $F(b) = F(x)|_{x=b}$, and so on.

Now, we can regard the value of $\tilde{\phi}^{(0)}$ obtained from (9.3.22) with Gregory correction (9.3.23) as the zeroth corrected approximation, which can be improved further to $\tilde{\phi}^{(1)}$ by computing

$$\tilde{\phi}_h^{(1)}(a+ih) - \lambda h \sum_{j=0}^n {}'' k(a+ih, a+jh) \tilde{\phi}_h^{(1)}(a+jh) = f(a+ih) + \lambda \delta_i \left(\tilde{\phi}^{(0)} \right). \quad (9.3.25)$$

In fact, if we write $\mathbf{d}^{(1)} = \tilde{\Phi}^{(1)} - \tilde{\Phi}^{(0)}$, we get

$$d_i^{(1)} - \lambda h \sum_{j=0}^n {}'' k(a+ih, a+jh) d_j^{(1)} = \lambda \delta_i \left(\tilde{\phi}^{(0)} \right),$$

which in matrix notation becomes

$$(\mathbf{I} - \lambda \mathbf{kD}) \mathbf{d}^{(1)} = \lambda \delta \left(\tilde{\Phi}^{(0)} \right).$$

Once $\mathbf{d}^{(1)}$ is computed, we obtain $\tilde{\Phi}^{(1)}$ from the relation $\tilde{\Phi}^{(1)} = \tilde{\Phi}^{(0)} + \mathbf{d}^{(1)}$. This scheme of computing $\tilde{\Phi}^{(1)}$ from $\tilde{\Phi}^{(0)}$ is known as *deferred correction* (see [Baker 1978](#), p.368).

9.3.5(b) Iterative Deferred Correction Scheme. Once we have computed $\tilde{\Phi}^{(1)}$ by the above correction scheme, we compute the vector $\tilde{\Phi}^{(i)}$, $i > 1$, such that

$$(\mathbf{I} - \lambda \mathbf{kD}) \mathbf{d}^{(i)} = \lambda \delta \left(\tilde{\Phi}^{(i-1)} \right), \quad (9.3.26)$$

where

$$\delta \left(\tilde{\Phi}^{(i-1)} \right) = \left[\delta_0 \left(\tilde{\Phi}^{(i-1)} \right), \delta_1 \left(\tilde{\Phi}^{(i-1)} \right), \dots, \delta_n \left(\tilde{\Phi}^{(i-1)} \right) \right]^T,$$

and $\delta_j \left(\tilde{\Phi}^{(i-1)} \right)$ is computed by substituting $\tilde{\Phi}^{(i-1)}$ for $\tilde{\Phi}$ in (9.3.24). Note that in (9.3.26) $\mathbf{k} = \left[k(a + ih, a + jh) \right]$, and $\mathbf{D} = \text{diag}(h/2, h, \dots, h, h/2)$, where \mathbf{I} is the identity matrix. To solve (9.3.26), we compute $\mathbf{d}^{(i)} = \tilde{\Phi}^{(i)} - \tilde{\Phi}^{(i-1)}$ at each stage for $i > 1$, such that $(\mathbf{I} - \lambda \mathbf{kD}) \mathbf{d}^{(i)} = \lambda \delta \left(\mathbf{d}^{(i-1)} \right)$, $i > 1$, which yields

$$\tilde{\Phi}^{(i)} = \tilde{\Phi}^{(i-1)} + \mathbf{d}^{(i)} = \mathbf{d}^{(1)} + \dots + \mathbf{d}^{(i)} + \tilde{\Phi}^{(0)},$$

where we compute $\delta \left(\mathbf{d}^{(i)} \right)$ for each next stage. This leads to the final desired approximation $\tilde{\Phi}^{(p)}$.

The above approximation scheme can also be constructed by using the Lagrangian form for $\delta_i \left(\tilde{\phi} \right)$; thus, in formula (9.3.24) we write

$$\delta_i \left(\tilde{\phi} \right) = h \sum_{j=0}^p \Omega_j^{[p]} \left\{ \vartheta_i(a + jh) + \vartheta_i(b - jh) \right\}, \tag{9.3.27}$$

where $\vartheta_i(x) = \vartheta_i \left(\tilde{\phi}; x \right)$, and some values of the coefficients $\Omega_j^{[p]}$ are tabulated below.

p	$j = 0$	$j = 1$	$j = 2$	$j = 3$
1	$-1/12$	$1/12$		
2	$-1/2$	$1/6$	$-1/24$	
3	$-109/720$	$177/720$	$-87/720$	$19/720$

Note that in the case when the matrix $(\mathbf{I} - \lambda \mathbf{kD})$ is ill conditioned, the vector $\mathbf{d}^{(i-1)}$, $i = 1, 2, \dots$, may be computed by Gaussian elimination followed by the above iterative scheme.

EXAMPLE 9.3.7. Let $k(x, s) = e^{xs}$, $f(x) = 1 - \frac{e^x - 1}{x}$, $0 \leq x \leq 1$, and $\lambda = 1$. The exact solution is $\phi(x) = 1$. The trapezoidal rule with Gregory’s correction is used. Baker (1978, p.370) has the following results:
(a) By a single deferred correction, the maximum errors are given in Table 9.3.7.

Table 9.3.7.

h	Trapezoidal	1 difference	2 differences	3 differences
1/8	2.42(−3)	2.97(−4)	4.22(−6)	1.33(−6)
1/16	6.0(−4)	3.81(−5)	3.63(−7)	4.54(−8)
1/32	1.50(−4)	4.85(−6)	2.81(−8)	1.81(−9)
1/64	3.75(−5)	6.13(−7)	2.42(−9)	6.86(−10)

(b) By iterative deferred correction, the maximum errors $\|\Phi - \tilde{\Phi}^{(i)}\|_\infty$ are:

h	Trapezoidal	1 iteration	2 iterations
1/8	1.6(−3)	2.2(−4)	1.0(−5)
1/16	4.0(−4)	3.0(−5)	7.6(−7)
1/32	1.1(−4)	1.2(−5)	1.4(−5)
1/64	3.7(−5)	2.0(−5)	2.0(−5)

No improvements over 2 iterations are obtained in 3, 4, or 5 iterations.

(c) By an iterative correction scheme using 5 differences (i.e., $p = 5$ in (9.3.24)), the values of $\tilde{\phi}$ are:

x	$h = 1/4$	$h = 1/8$	$h = 1/16$	Exact
± 1.0	1.64135	1.64011	1.63979	1.63970
± 0.75	1.75445	1.75258	1.75210	1.75195
± 0.5	1.84537	1.84313	1.84257	1.84238
± 0.25	1.90176	1.90040	1.89982	1.89962
± 0.0	1.92220	1.91982	1.91923	1.91903

These results are from Baker (1978, p.370ff). ■

EXAMPLE 9.3.8. (Baker 1978, p. 372) Consider

$$\phi(x) - \frac{1}{\pi} \int_0^1 \frac{\phi(s) ds}{1 + (x - s)^2} = 1.$$

Using the trapezoidal rule with step size $h = 1/32$ and the Gregory correction, the results are given in Table 9.3.8, where ‘iter(s)’ stands for the number of iterations.

Table 9.3.8.

x	trapezoidal	1 iter	2 iters	3 iters	4 iters	5 iters
0.0	1.918932	1.919033	1.919032	1.919031	1.919031	1.919031
0.25	1.899516	1.899616	1.899615	1.899615	1.899615	1.8996151
0.5	1.842291	1.842385	1.842384	1.842384	1.84238	1.8423847
0.75	1.751876	1.751954	1.751954	1.751995	1.751954	1.7519547
1.0	1.639643	1.639694	1.6396952	1.639695	1.639695	1.6396952 ■

9.3.6. Product Integration Method. We use quadrature rules when the integrand is the product of two functions. Accordingly, in the case of an integral equation we get

$$\int_a^b k(x,s)\phi(s) \, ds = \sum_{j=0}^n v_j \, k\left(x,s_j\right) \phi\left(s_j\right), \tag{9.3.28}$$

where the weights v_j are defined for various cases in §2.9. The above rule is exact when $\phi(x)$ is a polynomial of a certain degree on the interval $[a,b]$ or when $\phi(x)$ is a piece-wise polynomial of a certain degree on the subintervals $[a,a+h], [a+2h], \dots, [b-h]$. The approximation (9.3.28) permits us to apply the product integration rule to an FK2 of the form (9.1.2), which yields the approximation

$$\tilde{\phi}\left(x_i\right)-\lambda \sum_{j=0}^n v_j \, k\left(x_i,s_j\right) \tilde{\phi}\left(s_j\right)=f\left(x_i\right), \quad i=0,1, \ldots, n, \tag{9.3.29}$$

or in matrix form

$$\left(\mathbf{I}-\lambda \mathbf{K D}\right) \tilde{\Phi}=\mathbf{f}, \tag{9.3.30}$$

where \mathbf{I} is the identity matrix, $\mathbf{k}=\left(k\left(x_i,s_j\right)\right)_{ij}$, and $\mathbf{D}=\operatorname{diag}\left\{v_0, v_1, \ldots, v_n\right\}$. This method is exact for $\int_{-1}^1 k(x,s) \phi(s) \, ds$ if $k(x,s)$ is continuous and quadratic in each subinterval of $[-1,1]$. In the case when the kernel $k(x,s)$ is badly behaved at $s=x$, we use the rule (2.9.17), or its modifications.

EXAMPLE 9.3.9. Consider the same FK2 as in Example 9.3.6:

$$\phi(x)+\frac{1}{\pi} \int_{-1}^1 \frac{\phi(s)}{1+(x-s)^2} \, ds=1, \quad -1 \leq x \leq 1.$$

This equation in its general form

$$\phi(x)+\frac{1}{\pi} \int_{-1}^1 \frac{d}{d^2+(x-s)^2} \phi(s) \, ds=f(x), \quad |x| \leq 1,$$

was investigated by Young (1954a,b) by the product-integration method. His results are as follows:

x	0	$\pm 1/5$	$\pm 2/5$	$\pm 3/5$	$\pm 4/5$	± 1
$\tilde{\phi}(x)$	0.65741	0.66151	0.67389	0.69448	0.72249	0.75572

Compare these with the values of $\tilde{\phi}(x)$ in Example 9.3.6. The values of $\tilde{\phi}(x)$ using the trapezoidal rule with step size h are given below. This method gives better results for the amount of work involved. ■

x	0	$\pm 1/5$	$\pm 2/5$	$\pm 3/5$	$\pm 4/5$	± 1
$h = 0.1$	0.65787	0.66197	0.67432	0.69481	0.72261	0.75553
$h = 0.05$	0.65752	0.66163	0.67340	0.69546	0.72252	0.75567
$h = 0.025$	0.6574	0.66154	0.67392	0.69450	0.72249	0.75571
$h = 0.0125$	0.65742	0.66152	0.67389	0.69449	0.72249	0.75572

EXAMPLE 9.3.10. Consider an FK2 of the form $\phi(x) + \lambda \int_0^1 \kappa(x, s)g(s)\phi(s) \, ds = f(x)$, $0 \leq x \leq 1$, where $g(x) > 0$ for $0 \leq x \leq 1$ and $\frac{\partial \kappa(x, s)}{\partial s}$ has a discontinuity at $x = s$. An example is given by $\kappa(x, s) = \min\{x, s\}$, $0 \leq x \leq s \leq 1$, and $g(x) = e^x$. Because of the discontinuity in $\frac{\partial \kappa}{\partial s}$ in this problem, we do not use the quadrature rule (9.3.9) with $\varepsilon(x) = 0$, but instead use a quadrature rule of the form

$$\int_0^1 \min\{x, s\} \phi(s) \, ds = \sum_{j=0}^n v_j(x) \phi(jh), \tag{9.3.31}$$

and then find the solution of the system

$$\tilde{\phi}(ih) + \lambda \sum_{j=0}^n v_j(ih) g(jh) \tilde{\phi}(jh) = f(ih), \tag{9.3.32}$$

where we have $\lambda = 1$, $f(x) = 1.25 e^{2x} - 0.5 e^2 x - 0.25$, so that the equation has the exact solution $\phi(x) = e^x$. Baker (1978, p.385) has obtained the values of $\tilde{\phi}(x)$ given in Table 9.3.10, which are compared with the exact values. The results show an error of order $O(h^2)$.

Table 9.3.10.

h	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1.0$
1/10	1.2334	1.5158	1.8561	2.2665	2.7612
1/20	1.2245	1.4978	1.8306	2.2355	2.7292
1/40	1.2221	1.4933	1.8242	2.2280	2.7209
Exact	1.2214	1.4918	1.8221	2.2255	2.71828 ■

9.4. Singular Integral Equations

Singular integral equations occur (i) with a semi-infinite or infinite range; (ii) with a discontinuous derivative in either the kernel or the free term; (iii) with either an infinite or nonexistent derivative of some finite order; or (iv) any combination of these cases. Consider a singular equation of the second kind (SK2) of the form

$$(I + \lambda K)\phi(x) = f(x), \quad (9.4.1)$$

where K is the singular operator. Then

(a) Eq (9.4.1) has finitely many solutions $\{\phi_1(x), \dots, \phi_n(x)\}$.

(b) A necessary and sufficient condition for a solution of Eq (9.4.1) to exist is that $\int_{\Gamma} f(x) \psi_j(x) dx = 0$, where $\{\psi_1(x), \dots, \psi_m(x)\}$ is a maximal finite set of linearly independent solutions of the transposed homogeneous singular equation $(K^T \psi)(x) = 0$.

(c) The difference between the number n of linearly independent solutions of the homogeneous singular equation $(K\phi)(x) = 0$ and the number m of linearly independent solutions of the transposed homogeneous singular equation $(K^T \psi)(x) = 0$ depend only on the characteristic part of the operator K and is equal to its index, i.e., $n - m = \nu$ (for the for the definition of index ν , see [Muskhelishvili \(1992, p.90\)](#) and [Polyanin and Manzhirov \(1998, p.638\)](#)).

(d) The number of linearly independent solutions of characteristic equations is maximal among all singular equations with a given index ν . In particular, (i) if $\nu > 0$, then the homogeneous singular equation $(K_s \phi)(x) = 0$ has ν linearly independent solutions; (ii) if $\nu \leq 0$, then the homogeneous singular equation $(K\phi)(x) = 0$ has only the trivial solution; (iii) if $\nu \geq 0$, then the nonhomogeneous singular equation $(K_s \phi)(x) = f(x)$ has, in general, ν linearly independent solutions for an arbitrary function $f(x)$; and (iv) if $\nu < 0$, then the nonhomogeneous singular equation $(K_s \phi)(x) = f(x)$ is solvable iff $f(x)$ satisfies the $(-\nu)$ conditions $\int_{\Gamma} \Psi_j(x) f(x) dx = 0$, $j = 1, 2, \dots, -\nu$, where Γ is a simple closed contour, $\Psi_j(x) = x^{j-1}/Z(x)$, and $Z(x)$ denotes the fundamental solution of the homogeneous equation.

9.4.1. Singularities in Linear Equations. We consider the following cases:

CASE 1. The functions $k(x, s)$ and $f(x)$ are piecewise continuous, with jump discontinuities only along lines parallel to the coordinate axes. If the free term $f(x)$ is badly behaved, its form and nature of singularities are propagated into the solution $\phi(x)$. To remove this type of singularities, we write $\phi(x) = \psi(x) + f(x)$ and solve

the equation

$$\psi(x) = \lambda \int_a^b k(x, s)\psi(s) ds + \lambda \int_a^b k(x, s)f(s) ds. \quad (9.4.2)$$

Alternatively, we use a single function $\gamma(x)$ that has the ‘badness’ of $f(x)$ propagated into $\phi(x)$, and set $\phi(x) = \psi(x) + \gamma(x)$, so that $f(x) - \gamma(x)$ becomes well behaved. Then we use a quadrature rule to approximately solve for $\tilde{\psi}(x)$ the equation

$$\psi(x) - \lambda \int_a^b k(x, s)\psi(s) ds = [f(x) - \gamma(x)] + \lambda \int_a^b k(x, s)\gamma(s) ds, \quad (9.4.3)$$

which in turn yields $\tilde{\phi}(x)$. This method is successful only if $\int_a^b k(x, s)\psi(s) ds$ or $\int_a^b k(x, s)\gamma(s) ds$ are smooth functions of x , and especially if $k(x, s)$ is smooth.

CASE 2. If the function $f(x)$ behaves badly because of a discontinuity in a derivative, a high-order accuracy from a quadrature rule is not generally obtained since $\phi(x)$ may be affected by such behavior of $f(x)$.

CASE 3. Discontinuities in the kernel $k(x, s)$, which lie on lines parallel to the s -axis, pass on to the solution $\phi(x)$. In this case a quadrature rule or a collocation method is generally not applicable, but the product integration with a suitable choice of orthogonal polynomials $p_i(x)$ is needed to complete the solution in this case as well as in the case of the kernel of the form $k(x, s) = \frac{g(x, s)}{|s - s_1|^\alpha}$, $0 \leq \alpha < 1$.

CASE 4. When the kernel $k(x, s)$ is weakly singular, see §9.5.

CASE 5. Some special cases of the convolution-type kernels of singular integral equations of the form $k(x, s) = k(x - s)$ are as follows:

(i) If the interval of integration is $[a, \infty)$, we can apply the Fourier transforms to an FK1 or FK2, provided we assume that $f(x) < 0$ for $x < a$. Consider an FK1

$$\int_a^\infty k(x - s)\phi(s) ds = f(x). \quad (9.4.4)$$

The method described in Kythe and Puri (2002, p. 182) yields the solution for Eq (9.4.4), under the Dirichlet condition for $x > a$ and under the assumption that $\int_a^\infty |f(x)| dx < \infty$, as

$$\phi(x) = \begin{cases} \int_0^\infty d\mu \int_a^\infty \frac{\tilde{k}_c(\mu) \cos \pi\mu(s - x) + \tilde{k}_s(\mu) \sin \pi\mu(s - x)}{\tilde{k}_s^2(\mu) + \tilde{k}_c^2(\mu)} f(s) ds & \text{if } x > a, \\ 0 & \text{if } x < a, \end{cases}$$

where $\tilde{k}_c(\mu)$ and $\tilde{k}_s(\mu)$ denote the Fourier cosine and sine transforms of $k(x - s) = k(\tau)$, defined by

$$\tilde{k}_c(\mu) = \int_0^\infty k(\tau) \cos \pi\mu\tau d\tau, \quad \tilde{k}_s(\mu) = \int_0^\infty k(\tau) \sin \pi\mu\tau d\tau.$$

For $a = 0$, Eq (9.4.4) is known as the *Wiener-Hopf equation*.

(ii) If the interval of integration is (a, b) , then the solution for Eq (9.4.4) is similarly given by

$$\phi(x) = \int_{-\infty}^{\infty} d\eta \int_a^b \frac{\tilde{k}_c(\eta) \cos \pi\mu(s-x) + \tilde{k}_s(\eta) \sin \pi\mu(s-x)}{\tilde{k}_s^2(\eta) + \tilde{k}_c^2(\eta)} f(s) ds, \quad (9.4.5)$$

where

$$\tilde{k}_{c,s}(\eta) = \begin{cases} \int_{-\infty}^{\infty} k(\tau) \begin{cases} \cos & \text{if } a < x < b, \\ \sin & \end{cases} \pi\eta\tau d\tau \\ 0 & \text{if } x < a, b > x. \end{cases}$$

(iii) For an FK2 of the form

$$\phi(x) - \lambda \int_a^{\infty} k(x-s)\phi(s) ds = f(x), \quad (9.4.6)$$

the solution is

$$\phi(x) = \begin{cases} \int_0^{\infty} d\mu \int_a^{\infty} \frac{\tilde{k}_c(\mu) \cos \pi\mu(s-x) + \tilde{k}_s(\mu) \sin \pi\mu(s-x)}{\tilde{k}_s^2(\mu) + \tilde{k}_c^2(\mu) - \lambda [\tilde{k}_s^2 + \tilde{k}_c^2]} f(s) ds \\ \text{if } x > a, \\ 0 & \text{if } x < a. \end{cases} \quad (9.4.7)$$

(iv) If the interval of integration is $(-\infty, \infty)$, then by applying the convolution theorem of the Fourier integral the solution for an FK1 of the form $\int_{-\infty}^{\infty} k(x-s)\phi(s) ds = f(x)$ is given by

$$\phi(x) = \int_{-\infty}^{\infty} \tilde{\kappa}(x-s)f(s) ds, \quad (9.4.8)$$

where $\tilde{\phi}(u)$, $\tilde{k}(u)$, and $\tilde{f}(u)$ denote the Fourier transform of $\phi(x)$, $k(x)$, and $f(x)$, respectively, and $1/\tilde{k}(u) = \tilde{\kappa}(u)$. In the case of an FK2 of the form (9.4.6) the solution is given by

$$\phi(x) = f(x) - \lambda \int_{-\infty}^{\infty} k_{\lambda}(x-s)f(s) ds.$$

EXAMPLE 9.4.1. Consider the FK2 of the form (9.4.4) on the interval $(0, \infty)$. Divide the domain $x > 0, s > 0$ into four parts, marked by dotted lines $x = 1$ and $s = 1$, and let k_{11} , k_{12} , k_{21} , and k_{22} denote the values of the kernel $k(x-s)$ in these parts. Then the singular equation (9.4.4) becomes

$$\begin{aligned} \phi(x) - \lambda \left\{ \int_0^1 k_{11}(x,s)\phi(s) ds + \int_1^{\infty} k_{21}(x,s)\phi(s) ds \right. \\ \left. + \int_0^1 k_{12}(x,s)\phi(s) ds + \int_1^{\infty} k_{22}(x,s)\phi(s) ds \right\} = f(x). \end{aligned}$$

For the integral over the interval $(1, \infty)$, set $1/s = \sigma$; then, for example,

$$\int_1^\infty k_{21}(x, s)\phi(s) ds = \int_0^1 k_{21}\left(x, \frac{1}{\sigma}\right) \phi\left(\frac{1}{\sigma}\right) \frac{d\sigma}{\sigma^2}.$$

We then choose the nodes (lattice points) as, e.g., in Fig. 9.4.1 (see page 546), and solve the system of four simultaneous equations. For example, consider $k(x, s) = e^{-2(x+s)}$ and $f(x) = \frac{1}{x}$. We put $\frac{1}{x} = \xi$, $\frac{1}{s} = \sigma$, $\phi\left(\frac{1}{\xi}\right) = \Phi(\xi)$, $f\left(\frac{1}{\xi}\right) = F(\xi)$, and obtain

$$\Phi(\xi) - \int_0^1 \exp\left[-2\left(\frac{1}{\xi} + \frac{1}{\sigma}\right)\right] \Phi(\sigma) \frac{d\sigma}{\sigma^2} = \frac{\xi}{\xi + 1}.$$

Taking the four representative points (ξ, σ) as in Table 9.4.1, we have

$$\begin{aligned} 4.7\phi_1 + 3.4\phi_2 + 1.5\phi_3 + 1.2\phi_4 &= 9.0(+9), \\ 11.1\phi_1 + 7.1\phi_2 + 3.2\phi_3 + 2.4\phi_4 &= 3.0(+3), \\ 4.6\phi_1 + 3.4\phi_2 + 1.5\phi_3 + 1.1\phi_4 &= 4.0(+2), \\ 14.4\phi_1 + 10.5\phi_2 + 5.4\phi_3 + 3.6\phi_4 &= 5.0(+1). \end{aligned}$$

The solution is given in Table 9.4.1. For computational details, see [singular.nb](#) on the CD-R.

Table 9.4.1.

s	σ	ξ	$x = 1/\xi$	$\phi(x)$
0.15	6.67	0.8973	1.1145	-1.818(-10)
0.85	1.18	0.5938	1.6841	-7.733(-10)
1.18	0.85	0.4062	2.4615	-4.191(-10)
6.67	0.15	0.1029	9.7371	1.047(-10)

9.5. Weakly Singular Equations

For a weakly singular kernel of the form

$$k(x, s) = \frac{g(x, s)}{|x - s|^\alpha}, \quad 0 < \alpha < 1, \quad (9.5.1)$$

the resolvent is given by

$$k_\lambda(x, s) = \frac{D_\lambda(x, s)}{D(\lambda)}, \quad (9.5.2)$$

and the solution of the SK2 with a weakly singular kernel of the form (9.5.1) is given by

$$\phi(x) = f(x) + \lambda \int_a^b k_\lambda(x, s) f(s) ds. \quad (9.5.3)$$

For weakly singular equations the interpolatory quadrature rules described in [Chapter 2](#) are not applicable because $k(x, s)$ is unbounded if we assume that $g(x, s) \neq 0$ in (9.5.1). However, the product integration method can be used successfully for such equations. A modified quadrature method described in §9.3.2 can be extended to solve weakly singular equations. Since $k(x, s)$ is weakly singular, we have unbounded values in Eq (2.9.19). Let

$$\left\{ 1 + \lambda \Delta^*(s_j) \right\} \tilde{\phi}(s_i) - \lambda \sum_{\substack{j=0 \\ j \neq i}} v_j k(s_i, s_j) \tilde{\phi}(s_j) = f(s_i),$$

where

$$\Delta^*(s_i) = \sum_{\substack{j=0 \\ j \neq i}} v_j k(s_i, s_j) - \int_a^b k(s_i, s) ds.$$

Then we set $k(x, s) \{\phi(s) - \phi(x)\}$ to zero at the singularity $x = s$. Finally, from the computational point of view, the Galerkin or collocation methods are applicable to weakly singular equations (see [Baker 1978](#), p.532).

9.5.1. Product Integration Methods. In some problems the integral in an FK2 is singular in the sense that one or more derivatives of $k(x, s)$ have singularity within the interval of integration. In such a case we write $k(x, s) = u(x, s) \kappa(x, s)$, where $u(x, s)$ is singular in (a, b) and $\kappa(x, s)$ is a regular function of its arguments. It is assumed that this factorization of $k(x, s)$ is feasible; otherwise the method does not work. Moreover, u need not be unbounded at $x = s$ to create a singularity; u can be a function like $u(x, s) = \sqrt{x - s}$, where all derivatives with respect to s are unbounded at $x = s$, and p is thus singular in the above sense. Two examples of such integral equations are of the form

$$\phi(x) = f(x) + \lambda \int_a^b \frac{\kappa(x, s)}{|x - s|^\alpha} \phi(s) ds, \quad a < x < b, \quad 0 < \alpha < 1, \quad (9.5.4a)$$

$$\phi(x) = f(x) + \lambda \int_a^b \ln |x - s| \kappa(x, s) \phi(s) ds, \quad a < x < b. \quad (9.5.4b)$$

Thus, we write the FK2 as

$$\phi(x) = f(x) + \int_a^b u(x, s) \kappa(x, s) \phi(s) ds, \quad (9.5.5)$$

and to approximate its solution we use the product integration method; because of the singularity occurring in the kernel, this method is adapted to this situation by using the quadrature rules of §9.3.2 in the above two cases as follows.

CASE 1. When $k(x, s) = |x - s|^{-\alpha}$, $0 < \alpha < 1$, we take $\kappa(x, s) = 1$, and partition the interval $[a, b]$ into subintervals by choosing nodes $s_j = a + jh$, $h = (b - a)/n$, $j = 0, 1, \dots, n$. However, the points s_j need not be equally spaced. Then use the quadrature rule

$$\int_a^b k(x, s) \phi(s) ds = \sum_{j=0}^n v_j \phi(s_j),$$

where the weights v_j can be chosen as described in §2.9. This rule is exact if the function $\phi(x)$ is either piecewise constant in $[a, b]$, i.e., constant in each subinterval $[s_j, s_{j+1}]$, $j = 0, 1, \dots, n$, or continuous and piecewise linear in $[a, b]$, or a smooth function, i.e., a polynomial of degree n on $[a, b]$. Once we decide on the choice of the weights v_j , we apply the Nyström method and solve the system of algebraic equations

$$\tilde{\phi}(x_i) - \lambda \sum_{j=0}^n v_j \tilde{\phi}(s_j) = f(x_i), \quad i = 0, 1, \dots, n. \quad (9.5.6)$$

EXAMPLE 9.5.1. Consider the case of the weakly singular equation with the kernel $k(x, s) = |x - s|^{-1/2}$, for which we use the quadrature rule

$$\int_a^b \frac{1}{|x - s|^{1/2}} F(s) ds = \sum_{j=0}^n v_j(x_i) F(s_j),$$

where $F(x)$ is any function defined on $[a, b]$. This rule is an extension of the repeated trapezoidal rule, where the weights are taken as

$$\begin{aligned} v_0 &= \frac{1}{h} \int_{s_0}^{s_1} (s_1 - s) k(x_m, s) ds, \\ v_j &= \frac{1}{h} \left\{ \int_{s_{j-1}}^{s_j} (s - s_{j-1}) k(x_m, s) ds \right. \\ &\quad \left. + \int_{s_j}^{s_{j+1}} (s_{j+1} - s) k(x_m, s) ds \right\}, \quad j = 1, 2, \dots, n-1, \\ v_n &= \frac{1}{h} \int_{s_{n-1}}^{s_n} (s - s_{n-1}) k(x_m, s) ds, \end{aligned} \quad (9.5.7)$$

where $x_m = a + mh$. Thus, in this example, in order to compute v_j for $j = 0, 1, \dots, n$, we are required to compute

$$\frac{1}{h} \int_{s_{j-1}}^{s_j} \frac{(s_j - s) ds}{|s_m - s|^{1/2}} \quad \text{and} \quad \frac{1}{h} \int_{s_{j-1}}^{s_j} \frac{(s - s_{j-1}) ds}{|s_m - s|^{1/2}}.$$

ATKINSON’S TECHNIQUE. Atkinson (1976) suggests the following method to compute the above integrals: take $s = s_{j-1} + ht, 0 < t < 1$; then these integrals reduce to

$$h^{1/2} \int_0^1 \frac{1-t}{|q-t|^{1/2}} dt \quad \text{and} \quad h^{1/2} \int_0^1 \frac{t}{|q-t|^{1/2}} dt,$$

respectively, where $q = m - j + 1, -n + 1 \leq q \leq n$. Hence, we notice that these n^2 weights v_j are reduced to the above integrals with respect to t over $[0, 1]$, which can be computed analytically:

$$\begin{aligned} v_0 &= h^{1/2} \int_0^1 \frac{1-t}{|m-t|^{1/2}} dt, \\ v_j &= h^{1/2} \int_0^1 \frac{1-t}{|q-t|^{1/2}} dt, \quad j = 1, 2, \dots, n-1, \\ v_n &= h^{1/2} \int_0^1 \frac{1-t}{|m-n+1-t|^{1/2}} dt. \end{aligned} \tag{9.5.8}$$

Note that the weights v_j can be similarly evaluated for the logarithmic kernel $\ln |x-s|$ or any other difference kernel $k(x-s)$. ■

EXAMPLE 9.5.2. (Baker 1978, p.541) Consider the equation

$$\phi(x) - \lambda \int_{-1}^1 |x-s|^{-1/2} \phi(s) ds = f(x), \quad -1 \leq x \leq 1, \tag{9.5.9}$$

with $\lambda = 2/3$ and $f(x) = (1-x^2)^{3/4} - \frac{\pi}{2\sqrt{2}} (2-x^2)$. The exact solution is $\phi(x) = (1-x^2)^{3/4}$, which is not differentiable at $x = \pm 1$. We choose $s_j = jh - 1, h = 2/n$, and using the weights (9.5.8) we solve the system (9.5.6). The results for $n = 5$ are given in Table 9.5.2.

Table 9.5.2.

x	± 1.0	± 0.6	± 0.2
Error	$-2.55(-2)$	$2.25(-2)$	$1.27(-1)$

The rate of convergence is slow. The maximum error is as follows: $6.18(-2)$ for $n = 10$; $2.3(-2)$ for $n = 20$; $1.22(-2)$ for $n = 30$; $7.66(-3)$ for $n = 40$; $5.48(-3)$ for $n = 50$; $4.25(-3)$ for $n = 60$; and $3.42(-3)$ for $n = 70$. ■

Phillips (1969) uses a polynomial collocation method for solving Eq (9.5.9); he has calculated the accuracy both analytically and theoretically and obtained an error of about 3×10^{-2} with a polynomial of degree 7 (by solving a linear system of 8 equations) and an error of order $O(10^{-3})$ by solving a system of 30 equations.

CASE 2. When $k(x, s) = \ln |x - s|$, we may take, as in case 1, $\kappa(x, s) = 1$ and use the above method to solve the FK2. But instead, following Atkinson (1966), we choose $u(x, s) = |x - s|^{-1/2}$ and $\kappa(x, s) = |x - s|^{1/2} k(x, s)$. This choice of $\kappa(x, s)$ is continuous but not smooth for $0 \leq x, s \leq 1$, and $u(x, s)$ becomes unbounded at $s = x$. However, such a choice enables us to investigate the behavior of the method under bad computational conditions. Moreover, the method becomes very effective if we use trapezoidal rule (9.5.6) with weights defined by (9.5.8), that is,

$$\int_a^b \frac{1}{|x - s|^{1/2}} F(s) ds = \sum_{j=0}^n v_j F(s_j),$$

which leads to the system of equations

$$\tilde{\phi}(x_i) - \lambda \sum_{j=0}^n v_j \kappa(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad i = 0, 1, \dots, n. \quad (9.5.10)$$

EXAMPLE 9.5.3. Consider Eq (9.5.4b), where $\lambda = 1$, and

$$f(x) = x - \frac{1}{2} \left\{ x^2 \ln x + (1 - x^2) \ln(1 - x) - x - \frac{1}{2} \right\}.$$

The exact solution is $\phi(x) = x$. The system (9.5.10) becomes

$$\tilde{\phi}(x_i) - \sum_{j=0}^n v_j |x_i - s_j|^{1/2} \ln |x_i - s_j| \tilde{\phi}(s_j) = f(x_i),$$

or

$$(\mathbf{I} - \kappa \mathbf{D}) \tilde{\Phi} = \mathbf{f},$$

where $\kappa = (\kappa(x_i, s_j))_{ij}$, and $\mathbf{D} = \{v_0, v_1, \dots, v_n\}$. Using the 4-point trapezoidal rule we get $\tilde{\phi}_1 = 3.47916$, $\tilde{\phi}_2 = 0 = \tilde{\phi}_3$, and $\tilde{\phi}_4 = -4.74689$, which are very bad results. For computational details see [logkernel.nb](#) on the CD-R. ■

EXAMPLE 9.5.4. (Baker 1978, p.549) Let $k(x, s) = Y_0(|x - s|)$, where $Y_0(x)$ is the Bessel function of the second kind and order zero (also known as Weber's function of order zero). Note that

$$Y_0(x) = \frac{2}{\pi} \left[\ln \left(\frac{x}{2} \right) + \gamma \right] J_0(x) + \frac{2}{\pi} \left\{ \frac{x^2}{2^2} - \frac{x^4}{2^2 4^2} \left(1 + \frac{1}{2} \right) + \frac{x^6}{2^2 4^2 6^2} \left(1 + \frac{1}{2} + \frac{1}{3} \right) - \dots \right\},$$

where $J_0(x)$ is the Bessel function of the first kind and order zero. The function $Y_0(x)$ is unbounded at $x = 0$, so we take $u(x, s) = |x - s|^{-\alpha}$ and $\kappa(x, s) = |x - s|^\alpha Y_0(|x - s|)$. ■

BAKER'S METHOD. (Baker 1978, p.550) Consider an FK2 of the form (1.2.2) with $a = 0$ and $b = L$, and suppose that the kernel $k(x, s)$ is expressed in terms of complete elliptic integrals of the first and second kind; i.e., we take $k(x, s) = P(x, s) \ln |x - s| + Q(x, s)$, where $P(x, s) \in C[0, L]$ and $Q(x, s)$ has a singularity at $x = s$. The free term $f(x)$ is such that $\phi \in C[0, L]$. Baker (1978, p.559) mentions a work by Kershaw who solved this equation by using the quadrature rules

$$\begin{aligned} \int_0^L \ln |x - s| F(s) ds &= \sum_{j=0}^n v_{1,j} F(s_j), \\ \int_0^L Q(x, s) F(s) ds &= \sum_{j=0}^n v_{2,j} F(s_j), \quad s_j = jh, \quad h = L/n, \end{aligned} \quad (9.5.11)$$

where each rule is exact if $F(x)$ is piecewise polynomial. Then the approximate solution of the given FK2 is obtained by solving the system

$$\tilde{\phi}(x_i) - \lambda \sum_{j=0}^n \left\{ v_{1,j} P(x_i, s_j) + v_{2,j} \right\} \tilde{\phi}(s_j) = f(x_i).$$

This analysis lead to a general case when the kernel $k(x, s)$ can be represented by

$$k(x, s) = \sum_{m=0}^M k(x, s, m), \quad (9.5.12)$$

where $k(x, s, m)$ can be split as

$$k(x, s, m) = u(x, s, m) \kappa(x, s, m), \quad (9.5.13)$$

such that $\kappa(x, s, m) \in C[a, b]$ and $u(x, s, m)$ are weakly singular. Then we use the quadrature rule

$$\int_a^b u(x, s, m) F(s) ds = \sum_{j=0}^n v_{m,j} F(s_j),$$

which leads to the approximation formula

$$\tilde{\phi}(x_i) - \lambda \sum_{m=0}^M \sum_{j=0}^n v_{m,j} \kappa(x_i, s_j, m) \tilde{\phi}(s_j) = f(x_i).$$

Note that, in general, we will obtain different approximate values $\tilde{\phi}$ from different choices of the kernels $k(x, s, m)$ because its representation (9.5.12) is not explicit. Also, each function $k(x, s, m)$ may be written in many different ways as the product $u(x, s, m) \kappa(x, s, m)$.

EXAMPLE 9.5.5. (Atkinson 1966) Consider

(a) $k(x, s) = |x - s|^{-1/2} \kappa(x, s)$, where $\kappa(x, s) = |x - s|^{1/2} \ln |\cos x - \cos s| \in C[0, \pi]$, since if $\cos x = \cos s$, then $x = s + 2m\pi$, $m = 0, 1, 2, \dots$, and when $0 \leq x, s \leq \pi$, this implies $x = s$. This case satisfies all conditions except $\frac{\partial}{\partial s} \kappa(x, s)$ is unbounded at $x = s$. The results obtained, though poor, are given in Table 9.5.5a.

Table 9.5.5a.

n	$\phi_n(\pi/2)$	Error
4	0.59065	0.28
8	0.44853	0.13
16	0.38764	0.073
32	0.35347	0.38

(b) $k(x, s) = \ln |\cos x - \cos s|$, $0 \leq x, s \leq \pi$, which we can write in the form (9.5.12) with $M = 4$ as

$$\begin{aligned}\kappa_0(x, s) &= \ln \left\{ \frac{2 \sin \frac{x-s}{2}}{x-s} \right\}, \\ \kappa_1(x, s) &= \ln \left\{ \frac{2 \sin \frac{x-s}{2}}{(x+s)(2\pi-x-s)} \right\}, \\ \kappa_2(x, s) &= \kappa_3(x, s) = \kappa_4(x, s) = 1, \\ u_0(x, s) &= u_1(x, s)1, \\ u_2(x, s) &= \ln |x-s|, \\ u_3(x, s) &= \ln(2\pi-x-s), \\ u_4(x, s) &= \ln(x+s).\end{aligned}$$

Thus,

$$\begin{aligned}k(x, s) &= \ln |\cos x - \cos s| = \ln \left\{ \frac{\sin \frac{x-s}{2} \sin \frac{x+s}{2}}{\left(\frac{x-s}{2}\right)(x+s)(2\pi-x-s)} \right\} \\ &\quad + \ln |x-s| + \ln(2\pi-x-s) + \ln(x+s) \\ &= \sum_{m=1}^4 u_m(x, s) \kappa_m(x, s),\end{aligned}$$

where, as defined above, $u_m(x, s)$ are badly behaved whereas $\kappa_m(x, s)$ are regular. The exact solution of this equation is

$$\phi(x) = \frac{1}{1 + \pi \ln 2} \approx 0.314704298033644.$$

Using trapezoidal rule, Atkinson (1967) found the results given in Table 9.5.5b.

Table 9.5.5b.

n	$\phi_n(0)$	Error	Relative error
2	0.3051691	0.009535	3.029
4	0.3122181	0.002486	7.9(−1)
8	0.3140722	0.000632	2.0(−1)
16	0.3145453	0.000159	5.0(−2)
32	0.3146644	0.000039	1.267(−2)

Using Simpson’s rule, Atkinson (1967) found the results given in Table 9.5.5c.

Table 9.5.5c.

n	$\phi_n(0)$	Error	Relative error
2	0.32449048976	0.0002138	6.7(−2)
4	0.31468781777	0.00001648	5.2(−3)
8	0.31470316978	0.000001129	3.5(−4)
16	0.31470422550	0.000000073	2.3(−4)
32	0.31470429345	0.000000005	1.5(−6) ■

The representation (9.5.12) for the kernel $k(x, s)$ leads to an error of the order $O(h^3)$, but the error increases if $\phi(x)$ is badly behaved, or if one of the factors $\kappa_m(x, s)$ has a badly behaving derivative.

Atkinson achieves an error of $O(h^4)$ in the case of the kernel of Example 9.5.5. An error analysis for the product-integration method is provided by de Hoog and Weiss (1973b), who establish that the maximum local truncation errors at the nodes are $O(h^4 \ln h)$. In practice, the product-integration formulas mentioned above are not easy to use.

Atkinson (1972) has suggested a *hybrid method*, which is as follows: First, notice that the integrand with a singular kernel of the form (9.5.2) makes computational integration very difficult only when s is close to x . If we remove the disk $|s - x| \leq \delta$, $\delta > 0$, from the interval of integration $[a, b]$, then any one of the quadrature rules given in Chapters 2 and 3 can be used to approximate the solution over the interval $[a, s - \delta] \cup [s + \delta, b]$, where the quality of results will depend on δ . The integral over the remaining interval $(s - \delta, s + \delta)$ can then be handled by the product-integration methods, where we can take care of the singularity at $x = s$. For example, suppose that $s_0 = a$, $s_n = b$, and $s_j = s_{j-1} + h$; then set $\delta = h$ and use the repeated

trapezoidal rule, say, which gives

$$\begin{aligned}
 & \tilde{\phi}(x_i) - \lambda \frac{h}{2} \sum_{\substack{j=0 \\ j \neq i \\ j \neq i-1}} \left\{ k(x_i, s_j) \tilde{\phi}(s_j) + k(x_i, s_{j+1}) \tilde{\phi}(s_{j+1}) \right\} \\
 & - \lambda (1 - \delta_{i0}) \int_{x_{i-1}}^{x_i} \frac{1}{|x_i - s|^\alpha} \left\{ \frac{s - x_{i-1}}{h} g(x_i, x_i) \tilde{\phi}(x_i) \right. \\
 & \quad \left. + \frac{x_i - s}{h} g(x_i, s_{i-1}) \tilde{\phi}(s_{i-1}) \right\} \\
 & - \lambda (1 - \delta_{i0}) \int_{x_i}^{x_{i+1}} \frac{1}{|x_i - s|^\alpha} \left\{ \frac{s - x_i}{h} g(x_i, s_{i+1}) \tilde{\phi}(s_{i+1}) \right. \\
 & \quad \left. + \frac{x_{i+1} - s}{h} g(x_i, s_i) \tilde{\phi}(s_{j+1}) \right\} \\
 & + \frac{x_{i+1} - s}{h} g(x_i, s_j) \tilde{\phi}(s_j) = f(x_i), \quad i = 0, 1, \dots, n,
 \end{aligned}$$

where δ_{ij} is the Kronecker delta, and $k(x, s)$ is defined by (9.5.2).

9.5.2. Asymptotic Expansions. de Hoog and Weiss (1973b) derive a generalized Euler-Maclaurin formula for product integration based on piecewise Lagrangian interpolation, and derive asymptotic expansions for three cases of the function $u(x, s)$: (a) when $u(x, s)$ is regular; (b) when $u(x, s)$ is singular and of the form $|x - s|^\alpha$, $0 < \alpha < 1$, as in (9.5.4a); and (c) when $u(x, s)$ is of the form $\ln |x - s|$, as in (9.5.4b). Special cases of (b) and (c), i.e., $|\vartheta - s|^\alpha$ and $\ln |\vartheta - s|$, $0 \leq \vartheta \leq 1$, are also considered. Note that case (i) belongs to §9.5.1, so we shall present the formulas for cases (b) and (c) here.

Consider an SK2 of the form (9.5.5) with $a = 0$, $b = 1$, where the kernel is represented as

$$k(x, s) = \sum_{j=1}^n u_j(x, s) \kappa_j(x, s), \quad (9.5.14)$$

where the functions $u_j(x, s)$ and $\kappa_j(x, s)$ satisfy the following conditions:

- (i) $\kappa_j(x, s) \in C[0, 1]$;
- (ii) $\int_0^1 |u_j(x, s)| ds < +\infty$; and
- (iii) $\lim_{|x_1 - x_2| \rightarrow 0} \int_0^1 |u_j(x_1, s) - u_j(x_2, s)| ds = 0$ uniformly in x_1 and x_2 .

Special cases of $u_j(x, s)$ are mentioned above in (b) and (c). Therefore, we consider the special case $k(x, s) = u(x, s)\kappa(x, s)$. Choose the nodes for the interval $[0, 1]$ as $0 \leq s_1 < s_2 < \dots < s_n \leq 1$, and let $x_i = ih$ for $i = 0, 1, \dots, m$, $h = 1/m$.

We denote $x_{ij} = x_i + s_j h$ for $j = 1, 2, \dots, n$. Define

$$\pi(x) = \prod_{j=1}^n (x - s_j),$$

and the Lagrangian interpolating polynomials

$$l_j(x) = \frac{\pi(x)}{\pi'(s_j)(x - s_j)}, \quad j = 1, 2, \dots, n.$$

Then the computational scheme for the approximate solution $\tilde{\phi}$ of the FK2 is given by

$$\tilde{\phi}_{ij} = f(x_{ij}) + \lambda \sum_{l=0}^{m-1} \sum_{p=1}^n W_{lp} \kappa(x_{ij}, s_{lp}) \tilde{\phi}_{lp}, \quad (9.5.15)$$

for $i = 0, 1, \dots, m-1$; $j = 1, 2, \dots, n$, where

$$W_{lp}(x) = \int_{x_l}^{x_{l+1}} u(x, s) l_p \left(\frac{s - x_l}{h} \right) ds,$$

and $\tilde{\phi}_{ij}$ denotes the numerical approximation to $\phi(x_{ij})$. Atkinson (1967) shows that if λ is a regular value of the kernel, then (9.5.15) has a unique solution for sufficiently small h and $\max_{\substack{0 \leq i \leq m-1 \\ 1 \leq j \leq n}} |\phi(x_{ij}) - \tilde{\phi}_{ij}| = O(E)$, where the error

$$E = \max_{\substack{0 \leq i \leq m-1 \\ 1 \leq j \leq n}} \left| \sum_{l=0}^{m-1} \sum_{p=1}^n W_{lp} \kappa(x_{ij}, s_{lp}) \tilde{\phi}_{lp} - \int_0^1 k(x_{ij}, s) ds \right|.$$

The special cases for the error term are as follows:

When $u(x, s) = |\vartheta - x|^\alpha$, $0 < \vartheta < 1$, or $u(x, s) = |x - s|^\alpha$, $0 < \alpha < 1$,

$$E = O \left(h^n \int_0^1 \pi(s) ds \right) + O(h^{n+1-\alpha});$$

when $u(x, s) = \ln |\vartheta - x|$,

$$E = O \left(h^n \int_0^1 \pi(s) ds \right) + O(h^{n+1});$$

when $u(x, s) = \ln |x - s|$,

$$E = O \left(h^n \int_0^1 \pi(s) ds \right) + O(h^{n+1} \ln h).$$

The asymptotic expansions technique developed by Lyness and Ninham (1967) has been used to develop corresponding expansions for the two cases when $u(x, s)$ is singular. Thus, for the case when $u(x, s) = |x - s|^\alpha$ we have

$$\begin{aligned} h \sum_{l=0}^{m-1} |x_l + \vartheta h - s_{ij}|^\alpha \tilde{\phi}(x_l + \vartheta h) &= \int_0^1 |s - x_{ij}|^\alpha \\ &+ \sum_{q=0}^p \frac{h^{q+1}}{q!} \left\{ \hat{\zeta}(-q, \vartheta) \frac{d^q}{dx^q} (|x - x_{ij}|^\alpha \phi(s) ds) \Big|_{x=0} \right. \\ &+ (-1)^q \hat{\zeta}(-q, 1 - \vartheta) + \frac{d^q}{dx^q} (|x - x_{ij}|^\alpha \phi(s) ds) \Big|_{x=1} \left. \right\} \\ &+ \sum_{q=0}^p \frac{h^{q+1-\alpha}}{q!} \left[\hat{\zeta}(\alpha - q, \vartheta - s_j) + (-1)^q \hat{\zeta}(\alpha - q, 1 + s_j - \vartheta) \right] \phi^q(x_{ij}) \\ &+ O(x_{ij}^1 - \alpha \hat{h}^{p+1}) + O((1-x)^{1-\alpha} \hat{h}^{p+1}), \quad 0 < x_{ij} < 1, \quad p \geq 0, \end{aligned} \quad (9.5.16)$$

where $\hat{h} = h/x_{ij}$, and $\hat{\zeta}(\alpha, n)$ is the periodic zeta function defined by $\hat{\zeta}(\alpha, n) = \zeta(\alpha, \hat{\vartheta})$, $0 < \vartheta < 1$, such that $\vartheta - \hat{\vartheta}$ is an integer, and $\zeta(\alpha, x)$ is the generalized Riemann zeta function. Again, for the case when $u(x, s) = \ln|x - s|$, a formula similar to (9.5.16) holds except that the term $|x - x_{ij}|^\alpha$ is replaced by $\ln|x - x_{ij}|$ and the last two error terms are replaced by $O(\ln x_{ij} \bar{h}^{p+1}) + O(\ln(1 - x_{ij}) \bar{h}^{p+1})$, where $\bar{h} = h/(1 - x_{ij})$.

EXAMPLE 9.5.6. de Hoog and Weiss (1973b) consider the SK2

$$\phi(x) = 1 + \int_0^\pi \sum_{j=1}^4 u_j(x, s) \kappa_j(x, s) \phi(s) ds, \quad 0 \leq x \leq \pi,$$

where

$$\kappa_1(x, s) = \left\{ \frac{\sin((x-s)/2)}{((x-s)/2)} \right\} + \ln \left\{ \frac{\sin((x+s)/2)}{((x+s)(2\pi-x-s))} \right\},$$

$$u_2(x, s) = \ln|x - s|, \quad u_3(x, s) = \ln(2\pi - x - s),$$

$$u_4(x, s) = \ln(x + s), \quad u_1 = \kappa_2 + \kappa_3 = \kappa_4 = 1.$$

Compare this example with Example 9.5.5, where Atkinson (1967) applies the product Simpson's rule. Although the convergence rate was observed to be of the order $O(h^4)$, only $O(h^3)$ convergence was established. ■

9.5.3. Modified Quadrature Rule. A quadrature rule of the form

$$\int_a^b f(s) ds = \sum_{j=0}^n w_j f(s_j), \quad a \leq s_j \leq b, \quad j = 0, 1, \dots, n, \quad (9.5.17)$$

can be used to compute an approximate solution $\tilde{\phi}(x)$ of Eq (9.5.3) as follows: Write

$$\left\{1 - \lambda \int_a^b \frac{g(x, s)}{|x - s|^\alpha} ds\right\} \phi(x) - \lambda \int_a^b \frac{g(x, s)}{|x - s|^\alpha} [\phi(s) - \phi(x)] ds = f(x). \quad (9.5.18)$$

If $\phi \in H^\beta[a, b]$, where $\beta > \alpha$, the integrand in the second term on the left side tends to zero continuously as $x \rightarrow s$. The quadrature rule is then applicable and yields the approximate values $\tilde{\phi}(s_i)$, $i = 0, 1, \dots, n$, where

$$\left\{1 - \lambda G(s_i)\right\} \tilde{\phi}(s_i) - \lambda \sum_{\substack{j=0 \\ j \neq i}}^n \frac{g(s_i, s_j)}{|s_i - s_j|^\alpha} w_j [\tilde{\phi}(s_j) - \tilde{\phi}(s_i)] = f(s_i), \quad (9.5.19)$$

where

$$G(x) = \int_a^b \frac{g(x, s)}{|x - s|^\alpha} ds.$$

The values $\tilde{\phi}(s_i)$, $i = 0, 1, \dots, n$, will then define a function $\tilde{\phi}(x)$ by piecewise constant or piecewise linear interpolation if $a < s_0$ or $b > s_n$, or by polynomial or spline interpolation.

EXAMPLE 9.5.7. (Baker 1978, p.535) Let $k(x, s) = \ln|x + s|$, and define $g(x, s) = |x - s|^\alpha \ln|x + s|$, $0 < \alpha < 1$, and $g \in C[0, 1]$. Then $k(x, s) = \frac{g(x, s)}{|x - s|^\alpha} = \ln|x + s|$. The kernel $k(x, s)$ is weakly singular and square-integrable, i.e., $k(x, s) \in L_2[0, 1]$. For the SK2

$$\phi(x) - \int_0^1 \ln|x + s| \phi(s) ds = f(x), \quad 0 \leq x \leq 1, \quad (9.5.20)$$

we can use the modified quadrature rule (9.5.20) with

$$G(x) = \int_0^1 \ln|x + s| ds = (x + 1) \ln(x + 1) - x \ln x - 1.$$

The exact solution of Eq (9.5.20) is $\phi(x) = x$ if we take

$$f(x) = x + \frac{x^2}{2} \ln x - \frac{x^2}{4} - \frac{(x + 1)^2}{2} \ln(x + 1) + \frac{(x + 1)^2}{4},$$

which corresponds to $G(x)$. This modified quadrature rule is applied using the

- (a) $(n + 1)$ -point repeated midpoint rule,
- (b) n -times repeated trapezoidal rule, and
- (c) repeated Simpson's rule with $(n + 1)$ points.

The results are given in Table 9.5.7 for different values of n (Baker 1978, p.535). The error seems to be of the order $O(h^2 \ln h)$. ■

Table 9.5.7.

n	(a)	(b)	(c)
2	1.16(−2)	5.52(−2)	1.16(−2)
4	4.27(−3)	1.37(−2)	3.45(−3)
8	1.34(−3)	3.43(−3)	9.74(−4)
16	4.31(−4)	1.05(−3)	2.64(−4)
32	1.33(−4)	3.14(−3)	6.95(−5)
64	3.98(−5)	9.18(−5)	1.80(−5)
128	1.16(−5)	2.64(−5)	4.58(−6)

EXAMPLE 9.5.8. Consider the FK2

$$\phi(x) - \int_0^1 \ln|x-s| \phi(s) ds = f(x), \quad 0 \leq x \leq 1, \quad (9.5.21)$$

whose exact solution is $\phi(x) = x$ for

$$f(x) = x - \frac{1}{2} \left\{ x^2 \ln x + (1+x^2) \ln(1-x) - \left(x + \frac{1}{2} \right) \right\}.$$

Using the modified rule (9.5.21) with the repeated Simpson's rule, we compute $\tilde{\phi}(x)$ for different step sizes h . The results are given in Table 9.5.8 (see Baker 1978, p.537).

Table 9.5.8.

$h \setminus x$	0.0	0.25	0.5	0.75	1.0
1/2	−1.3(−2)		3.6(−12)		1.3(−2)
1/4	−3.6(−3)	7.5(−5)	3.6(−12)	−7.5(−5)	3.6(−3)
1/8	−1.0(−3)	1.9(−5)	7.3(−12)	−1.9(−5)	1.0(−4)
1/16	−2.7(−4)	3.1(−6)	−1.5(−11)	−3.1(−6)	2.7(−4)
1/32	−7.1(−5)	4.4(−7)	7.3(−12)	−4.4(−7)	7.1(−5)
1/64	−1.8(−5)	5.8(−8)	−2.2(−11)	−5.8(−8)	1.8(−5)

The values at $x = 0.5$ are correct up to the level of roundoff error; the maximum error occurs at $x = 0$ and $x = 1$, and the rate of decrease is that of order $O(h^2 \ln h)$ as h decreases. The errors at the points $x = 0.25$ and $x = 0.75$ decrease faster than the above order. ■

9.6. Cauchy Singular Equations of the First Kind

A Cauchy singular equation of the first kind (CSK1) is defined in the complex plane \mathcal{C} by

$$\frac{1}{i\pi} \oint_{\Gamma} \frac{\phi(\zeta)}{\zeta - z} d\zeta = f(z), \quad (9.6.1)$$

where Γ is a closed or nonclosed contour in \mathcal{C} with $z = x + iy$, and ζ and z are (complex) points on Γ , $\phi(z)$ is the unknown function, $\frac{1}{\zeta - z}$ is the Cauchy kernel, and $f(z)$ is the free term. The integral on the left side of Eq (9.6.1) exists only as the Cauchy p.v. If Γ is a closed contour, special cases of Eq (9.6.1) are the following:

(i) A CSK1 on the real axis has the form

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x} ds = f(x), \quad -\infty < x < \infty. \quad (9.6.2)$$

(ii) A CSK1 on a finite interval $[a, b]$ has the form

$$\frac{1}{\pi} \int_a^b \frac{\phi(s)}{s - x} ds = f(x), \quad a \leq x \leq b < \infty. \quad (9.6.3)$$

In Eqs (9.6.1)–(9.6.3) it is assumed that all functions satisfy the Hölder condition. A general form of a CSK1 in \mathcal{C} is

$$\frac{1}{i\pi} \oint_{\Gamma} \frac{g(z, \zeta)}{\zeta - z} d\zeta = f(z),$$

where $g(z, \zeta)$ is a given function that satisfies the Hölder condition with respect to both variables, and all other functions satisfy the Hölder condition as in Eqs (9.6.1)–(9.6.3).

If in Eq (9.6.1) we replace the variable z by ζ_1 , multiply by $\frac{1}{i\pi} \frac{d\zeta_1}{\zeta_1 - z}$, integrate along Γ , and change the order of integration by using the Poincaré-Betrand formula (1.1.7) with $g(z, z) = \phi(z)$ in this case, then we obtain

$$\frac{1}{i\pi} \oint_{\Gamma} \frac{f(\zeta_1) d\zeta_1}{\zeta_1 - z} = \phi(z) + \frac{1}{i\pi} \int_{\Gamma} \phi(\zeta) d\zeta \cdot \frac{1}{i\pi} \oint_{\Gamma} \frac{d\zeta_1}{(\zeta_1 - z)(\zeta - \zeta_1)},$$

where the second integral on the right side for a closed contour Γ is

$$\oint_{\Gamma} \frac{d\zeta_1}{(\zeta_1 - z)(\zeta - \zeta_1)} = \frac{1}{\zeta - z} \left(\oint_{\Gamma} \frac{d\zeta_1}{\zeta_1 - \zeta} - \oint_{\Gamma} \frac{d\zeta_1}{\zeta_1 - z} \right) = \frac{1}{\zeta - z} (i\pi - i\pi) = 0.$$

Hence, the solution of Eq (9.6.1) for a closed contour Γ is

$$\phi(z) = \frac{1}{i\pi} \oint_{\Gamma} \frac{f(\zeta)}{\zeta - z} d\zeta.$$

9.6.1. Use of Trigonometric Polynomials. Consider a CSK1 on the interval $[-1, 1]$ defined by

$$\frac{1}{\pi} \oint_{-1}^1 \frac{\phi(s)}{s - x} ds + \frac{1}{\pi} \int_{-1}^1 k(x, s) \phi(s) ds = f(x). \quad (9.6.4)$$

This equation is encountered in problems of aerodynamics and plane elasticity (see [Kalandiya 1973](#)). We consider the following three cases.

CASE 1. SOLUTION UNBOUNDED AT EACH ENDPOINT. According to [Mushkelishvili \(1992\)](#), this solution is of the form

$$\phi(x) = \frac{g(x)}{\sqrt{1 - x^2}}, \quad (9.6.5)$$

where $g(x)$ is a bounded function on $[-1, 1]$. Substituting (9.6.5) into Eq (9.6.4) and setting $x = \cos \theta$, $s = \cos \sigma$, $0 \leq \theta, \sigma \leq \pi$, we get

$$\frac{1}{\pi} \oint_{-1}^1 \frac{g(\cos \sigma)}{\cos \sigma - \cos \theta} d\sigma + \frac{1}{\pi} \int_{-1}^1 k(\cos \theta, \cos \sigma) g(\cos \sigma) d\sigma = f(\cos \theta).$$

We replace the function $g(x)$ by the Lagrange interpolation polynomials l_n with Chebyshev nodes $x_m = \cos \theta_m$, $\theta_m = \frac{2m-1}{2n} \pi$, $m = 1, \dots, n$, where

$$l_n(g; \cos \theta) = \frac{1}{n} \sum_{j=1}^n (-1)^{j+1} g(\cos \theta_j) \frac{\cos n\sigma \sin \theta_j}{\cos \theta - \cos \theta_j}. \quad (9.6.6)$$

For each j the fraction on the right side of (9.6.6) is an even trigonometric polynomial of degree $\leq (n-1)$, and

$$\frac{1}{\pi} \int_0^\pi \frac{\cos n\sigma}{\cos \sigma - \cos \theta} d\sigma = \frac{\sin n\theta}{\sin \theta}, \quad n = 0, 1, 2, \dots$$

We write (9.6.6) as

$$l_n(g; \cos \theta) = \frac{2}{n} \sum_{j=1}^n g(\cos \theta_j) \sum_{m=0}^{n-1} \cos \theta_j \cos m\theta - \frac{1}{n} \sum_{j=1}^n g(\cos \theta_j).$$

Then we obtain the following quadrature rule for the singular part of Eq (9.6.4):

$$\frac{1}{\pi} \oint_{-1}^1 \frac{\phi(s)}{s - x} ds = \frac{2}{n \sin \theta} \sum_{j=1}^n g(\cos \theta_j) \sum_{m=1}^{n-1} \cos m\theta_m \sin m\theta. \quad (9.6.7)$$

This formula is exact only in the case when $g(s)$ is a polynomial of degree $\leq (n-1)$.

For the second integral (regular part) on the left side of Eq (9.6.4) we use the relation

$$\frac{1}{\pi} \int_{-1}^1 \frac{P(x) dx}{\sqrt{1-x^2}} = \frac{1}{n} \sum_{j=1}^n P(\cos \theta_j),$$

where $P(x)$ is a polynomial of degree $\leq (2n-1)$. Then

$$\frac{1}{\pi} \int_{-1}^1 k(x, s) \phi(s) ds = \frac{1}{n} \sum_{j=1}^n k(\cos \theta, \cos \theta_j) g(\cos \theta_j). \quad (9.6.8)$$

Thus, substituting (9.6.7) and (9.6.8) into Eq (9.6.4), we get

$$\begin{aligned} \frac{2}{n \sin \theta} \sum_{j=1}^n g(\cos \theta_j) \sum_{m=1}^{n-1} \cos m \theta_j \sin m \theta + \frac{1}{n} \sum_{j=1}^n k(\cos \theta, \cos \theta_j) g(\cos \theta_j) \\ = f(\cos \theta). \end{aligned} \quad (9.6.9)$$

If we set $\theta = \theta_i$, $i = 1, \dots, n$, and use the relation

$$\sum_{m=1}^{n-1} \cos m \theta_j \sin m \theta_i = \frac{1}{2} \cot \frac{\theta_i \pm \theta_j}{2}, \quad (9.6.10)$$

where the \pm sign is chosen according as $|i-j|$ is even or odd, we obtain from (9.6.9) the following system of linear algebraic equations:

$$\begin{aligned} \sum_{j=1}^n a_{ij} g_j = f_i, \quad f_i = f(\cos \theta_i), \quad i = 1, \dots, n, \\ a_{ij} = \frac{1}{n} \left[\csc \theta_i \cot \frac{\theta_i \pm \theta_j}{2} + k(\cos \theta_i, \cos \theta_j) \right], \end{aligned}$$

which determines the approximate values of $g_j = g(\cos \theta_j)$. This solution for g_j is then substituted into (9.6.6) and (9.6.5) to obtain the approximate solution $\tilde{\phi}$ of Eq (9.6.4) at the nodes x_j .

CASE 2. SOLUTION BOUNDED AT ONE ENDPOINT. Let the solution be bounded at the endpoint $x = -1$. Then we take

$$\phi(x) = \sqrt{\frac{1-x}{1+x}} h(x), \quad (9.6.11)$$

where $h(x)$ is bounded on $[-1, 1]$. We choose the same interpolation nodes as in Case 1, replace $h(x)$ by the trigonometric polynomial

$$l_n(h; \cos \theta) = \frac{1}{n} \sum_{j=1}^n (-1)^{j+1} h(\cos \theta_j) \frac{\cos n \theta \sin \theta_j}{\cos \theta - \cos \theta_j}, \quad (9.6.12)$$

and substitute the result into the singular part of Eq (9.6.4). This gives the following quadrature rule for the singular part of Eq (9.6.4):

$$\frac{1}{\pi} \int_{-1}^1 \frac{\phi(s)}{s-x} ds = 2 \frac{1-\cos\theta}{n \sin\theta} \sum_{j=1}^n h(\cos\theta_j) \sum_{m=1}^{n-1} \cos m\theta_j \sin m\theta - \frac{1}{n} \sum_{j=1}^n h(\cos\theta_j), \quad (9.6.13)$$

which is exact only if $h(s)$ is a polynomial of degree $\leq (n-1)$. The quadrature rule for the regular part of Eq (9.6.4) is

$$\frac{1}{\pi} \int_{-1}^1 k(x,s) \phi(s) ds = \frac{1}{n} \sum_{j=1}^n (1-\cos\theta_j) k(\cos\theta, \cos\theta_j) h(\cos\theta_j), \quad (9.6.14)$$

which is exact only if the integrand is a polynomial of degree $\leq (2n-2)$. Now, after substituting (9.6.13) and (9.6.14) into Eq (9.6.4) and using $\theta = \theta_i$ ($i = 1, \dots, n$) and the relation (9.6.10), we obtain the following system of algebraic equations:

$$\sum_{j=1}^n b_{ij} h_j = f_i, \quad f_i = f(\cos\theta_i), \quad i = 1, \dots, n, \\ b_{ij} = \frac{1}{n} \left[\tan \frac{\theta_i}{2} \cot \frac{\theta_i \pm \theta_j}{2} - 1 + 2 \sin^2 \frac{\theta_j}{2} k(\cos\theta_i, \cos\theta_j) \right],$$

which determines the approximate value $h_j = h(\cos\theta_j)$. This solution for h_j is then used in (9.6.12) and (9.6.11) to obtain the approximate solution $\tilde{\phi}$ of Eq (9.6.4) at the nodes x_j .

Note that if the solution is unbounded at the other endpoint $x = 1$, we take

$$\phi(x) = \sqrt{\frac{1+x}{1-x}} h(x).$$

CASE 3. SOLUTION BOUNDED AT BOTH ENDPOINTS. In this case the solution $\phi(x)$ must satisfy the boundary conditions $\phi(-1) = 0 = \phi(1)$. We approximate $\phi(x)$ by an even trigonometric polynomial in θ , which is constructed for the nodes $x_j = \cos\theta_j$ of the corresponding Chebyshev polynomial of the second kind, namely, by

$$M_n(\phi; \cos\theta) = \frac{2}{n+1} \sum_{j=1}^n \phi(\cos\theta_j) \sum_{m=1}^n \sin m\theta_j \sin m\theta. \quad (9.6.15)$$

This leads to the following quadrature rule for the singular part of Eq (9.6.4):

$$\frac{1}{\pi} \int_{-1}^1 \frac{\phi(s)}{s-x} ds = -\frac{2}{n+1} \sum_{j=1}^n \phi(\cos\theta_j) \sum_{m=1}^n \sin m\theta_j \cos m\theta, \quad (9.6.16)$$

which is exact for any odd trigonometric polynomial ϕ of degree $\leq n$. For the regular part of Eq (9.6.4) we use the relation

$$\int_{-1}^1 \sqrt{1-x^2} P(x) dx = \frac{\pi}{n+1} \sum_{j=1}^n \sin^2 \theta_j P(\cos \theta_j), \quad (9.6.17)$$

where $P(x)$ is a polynomial of degree $\leq (2n-1)$, as in Case 1. Thus, in view of (9.6.17), the quadrature rule for the regular part of Eq (9.6.4) is

$$\frac{1}{\pi} \int_{-1}^1 k(x, s) \phi(s) ds = \frac{1}{n+1} \sum_{j=1}^n \sin \theta_j k(\cos \theta, \cos \theta_j) \phi(\cos \theta_j). \quad (9.6.18)$$

Now, after we substitute (9.6.16) and (9.6.18) into Eq (9.6.4) and set $\theta = \theta_i, i = 1, \dots, n$, we obtain the following system of algebraic equations:

$$\begin{aligned} \sum_{j=1}^n c_{ij} h_j &= f_i, \quad f_i = f(\cos \theta_i), \quad i = 1, \dots, n, \\ c_{ij} &= \frac{\sin \theta_j}{n+1} \left[\frac{2e_{ij}}{\cos \theta_j - \cos \theta_i} + k(\cos \theta_i, \cos \theta_j) \right], \\ e_{ij} &= \begin{cases} 0 & \text{for even } |i-j|, \\ 1 & \text{for odd } |i-j|. \end{cases} \end{aligned}$$

Once this system is solved for $h_j = h(\cos \theta_j)$, the approximate solution $\tilde{\phi}$ is computed from (9.6.15). When using this method, it is important to have the approximate solution of the form

$$\tilde{\phi}(x) = (1-x)^\alpha (1+x)^\beta \Psi(x), \quad (9.6.19)$$

where $\alpha = \pm 1/2 = \beta$, and $\Psi(x)$ is a bounded function on the interval $[-1, 1]$ with well-defined values $\Psi(-1)$ and $\Psi(1)$. If the representation (9.6.19) holds, then this method is also applicable to Cauchy singular integral equations of the second kind (CSK2) discussed next.

9.7. Cauchy Singular Equations of the Second Kind

A singular equation of the second kind with a Cauchy kernel (CSK2) is generally of the form

$$a(x) \phi(x) + \frac{b}{i\pi} \oint_{\Gamma} \frac{g(x, s)}{s-x} \phi(s) ds = f(x), \quad (9.7.1)$$

where Γ is a closed or nonclosed contour, and s and x are points on Γ . It is assumed that the functions $a(x)$, $\phi(x)$, and $f(x)$ satisfy the Hölder condition on Γ and the function $g(x, s)$ also satisfies the Hölder condition on Γ with respect to both variables. The kernel of Eq (9.7.1) can be written as

$$\frac{g(x, s)}{s - x} = \frac{g(x, s) - g(x, x)}{s - x} + \frac{g(x, x)}{s - x} = f(x),$$

and if we set $g(x, x) = b(x)$ and $\frac{g(x, s) - g(x, x)}{s - x} = i\pi k(x, s)$, then Eq (9.7.1) takes the form

$$a(x)\phi(x) + \frac{b(x)}{i\pi} \oint_{\Gamma} \frac{\phi(s)}{s - x} ds + \int_{\Gamma} k(x, s)\phi(s) ds = f(x), \quad (9.7.2)$$

where $b(x)$ satisfies the Hölder condition on Γ , and $k(x, s)$ satisfies the Hölder condition everywhere on Γ except at the points $s = x$, where we have $|k(x, s)| < A|s - x|^{-\alpha}$, A a positive constant, and $0 \leq \alpha < 1$. Eq (9.7.2) is taken as the standard form of a CSK2, where $a(x)$ and $b(x)$ are called the coefficients of the equation, $\frac{1}{s - x}$ the Cauchy kernel, $k(x, s)$ the kernel of the regular part, and $f(x)$ the free term. The first term on the left side of Eq (9.7.2) is also known as the *characteristic part* of the equation.

Eqs (9.7.1) and (9.7.2) can be written in the operator form as

$$(K\phi)(x) \equiv (K_s + K_r)(x) = f(x), \quad (9.7.3)$$

where $K = K_s$ is known as the *singular operator* such that the equation

$$(K_s\phi)(x) \equiv a(x)\phi(x) + \frac{b(x)}{i\pi} \oint_{\Gamma} \frac{\phi(s)}{s - x} ds = f(x) \quad (9.7.4)$$

is called the *characteristic equation* for Eq (9.7.2), and the operator K_s is sometimes called the *characteristic operator*. For the regular part of Eq (9.7.2) we have

$$(K_r\phi)(x) \equiv \int_{\Gamma} k(x, s)\phi(s) ds,$$

where K_r is called the *regular (Fredholm) operator*. Thus, Eq (9.7.2) can be written as

$$(K\phi)(x) \equiv (K_s\phi)(x) + (K_r\phi)(x) = f(x). \quad (9.7.5)$$

The equation

$$(K^T\phi)(x) \equiv a(x)\phi(x) - \frac{1}{i\pi} \oint_{\Gamma} \frac{b(s)\phi(s)}{s - x} ds + \int_{\Gamma} k(s, x)\phi(s) ds = g(x) \quad (9.7.6)$$

is the *transposed* CSK2, where K^T is the transposed operator of the operator K . The equation

$$\left((K_s)^T \phi\right)(x) \equiv a(x)\phi(x) - \frac{1}{i\pi} \int_{\Gamma} \frac{b(s)\phi(s)}{s-x} ds = g(x) \quad (9.7.7)$$

is the *transposed characteristic equation* to Eq (9.7.4). Note that $(K_s)^T \neq (K^T)_s$, where

$$\left((K^T)_s \phi\right)(x) \equiv a(x)\phi(x) - \frac{b(x)}{i\pi} \int_{\Gamma} \frac{\phi(s)}{s-x} ds. \quad (9.7.8)$$

Some examples of CSK2 include the following:

(a) Consider the CSK2

$$a\phi(x) + \frac{b}{\pi} \int_{-1}^1 \frac{\phi(s) ds}{s-x} = f(x), \quad -1 < x < 1,$$

where, without loss of generality, we can take $a^2 + b^2 = 1$. We have three cases:

(i) Solution bounded at both endpoints:

$$\phi(x) = a f(x) - \frac{b}{\pi} \int_{-1}^1 \frac{g(s)}{g(s)} \frac{f(s) ds}{s-x}, \quad (9.7.9)$$

where $g(x) = (1+x)^\alpha(1-x)^{1-\alpha}$, and α is a root of the equation

$$a + b \cot(\pi\alpha) = 0 \quad (9.7.10)$$

on the interval $0 < \alpha < 1$. The above solution exists iff $\int_{-1}^1 \frac{f(s)}{g(s)} ds = 0$.

(ii) Solution bounded at the endpoint $x = 1$ and unbounded at $x = -1$ is given by (9.7.9) with $g(x) = (1+x)^\alpha(1-x)^{-\alpha}$, where in this case α is the root of Eq (9.7.10) on the interval $-1 < \alpha < 0$.

(iii) Solution unbounded at both endpoints:

$$\phi(x) = a f(x) - \frac{b}{\pi} \int_{-1}^1 \frac{g(s)}{g(s)} \frac{f(s) ds}{s-x} + C g(x),$$

where $g(x) = (1+x)^\alpha(1-x)^{-1-\alpha}$, C is an arbitrary constant, and α is a root of Eq (9.7.10) on the interval $0 < x < 1$.

(b) Tricomi equation

$$\phi(x) - \lambda \int_0^1 \left(\frac{1}{s-x} - \frac{1}{x+s-2xs} \right) \phi(s) ds = f(x), \quad 0 < x < 1,$$

has the solution

$$\phi(x) = \frac{1}{1 + \lambda^2 \pi^2} \left[f(x) + \int_0^1 \left(\frac{1}{s-x} - \frac{1}{x+s-2xs} \right) f(s) ds \right] + \frac{C(1-x)^\beta}{x^{1+\beta}},$$

where C is an arbitrary constant, and

$$\begin{aligned} \alpha &= \frac{2}{\pi} \tan^{-1}(\lambda\pi), \quad -1 < \alpha < 1, \\ \beta &= \frac{2}{\pi} \tan^{-1}(\lambda\pi), \quad -2 < \beta < 0. \end{aligned}$$

Eq (9.7.1) can be solved in a closed form if $a(x) = a$ and $b(x) = b$ are constants and the kernel $k(x, s)$ is analytic in each variable in the domain $\Omega^+ = \text{Int}(\Gamma)$, where Γ is the (closed) boundary of this domain. Then Eq (9.7.1) becomes

$$a\phi(x) + \frac{1}{i\pi} \oint_{\Gamma} \frac{g(x, s)}{s-x} \phi(s) ds = f(x),$$

where $g(x, s) = b - i\pi k(x, s)$, and the solution is given by

$$\phi(x) = \frac{1}{a^2 - b^2} \left[f(x) - \frac{1}{i\pi} \oint_{\Gamma} \frac{g(x, s)}{s-x} f(s) ds \right], \quad a \neq \pm b.$$

9.7.1. Gauss-Jacobi Quadrature. Erdogan and Gupta (1972), Erdogan, Gupta and Cook (1973), and Krenk (1975) show that by a proper choice of collocation points both CSK1 and CSK2 can be solved using the Gauss-Jacobi quadrature rule. Consider a CSK2 in its general form

$$a_i \phi_i(x) + \frac{b_i}{\pi} \int_{-1}^1 \phi_i(s) \frac{ds}{s-x} + \lambda \sum_{i=1}^N \int_{-1}^1 k_{ij}(x, s) \phi(s) ds = f_i(x), \quad |x| < 1, \quad (9.7.11)$$

for $j = 1, \dots, N$, where a_i and b_i are real constants, the kernels $k_{ij}(x, s) \in H([-1, 1])$, and the free terms $f_i(x)$ are known functions. The unknown functions $\phi_i(x)$ or their first derivatives have integrable singularities at the endpoints $x = \pm 1$. A general closed-form solution of Eq (9.7.11) is not known. However, for numerical solution based on the Gauss-Jacobi quadrature rule Erdogan, Gupta and Cook (1973) have found a group of fundamental functions defined by

$$w_i(x) = (1-x)^{\alpha_j} (1+x)^{\beta_j}, \quad (9.7.12)$$

where

$$\begin{aligned} \alpha_j &= \frac{1}{2i\pi} \log \frac{a_j - ib_j}{a_j + ib_j} + N_j, \\ \beta_j &= -\frac{1}{2i\pi} \log \frac{a_j - ib_j}{a_j + ib_j} + M_j, \end{aligned}$$

N_j and M_j being integers for $j = 1, \dots, N$, and for each of the N equations in (9.7.11) the index κ_j of the integral operators K_{ij} is defined by

$$\kappa_j = -(\alpha_j + \beta_j) = -(N_j + M_j), \quad j = 1, \dots, N.$$

Since we have assumed that ϕ_i or their first derivatives have integrable singularities at the endpoints, the index must be $-1, 0, 1$ (see Mushkhelishvili 1992). The numerical solution of Eq (9.7.11) is given by

$$\phi_i(x) = g_i(x) w_i(x),$$

where

$$g_i(x) = \sum_{i=1}^{\infty} c_{ij} P_j^{(\alpha, \beta)}(x). \quad (9.7.13)$$

Here $P_n^{(\alpha, \beta)}(x)$ are Jacobi polynomials of degree n with indices α and β , and c_{ij} are constants to be determined. The general scheme is to truncate the series (9.7.13) for $i = 1, \dots, n$, and determine methods to compute the unknown coefficients c_{ij} . We discuss this problem below for a simple case of Eq (9.7.11), but the method can be easily extended to Eq (9.7.11).

9.7.2. Solution by Jacobi Polynomials. For the sake of simplicity we consider a special case of Eq (9.7.11) of the form

$$a \phi(x) + \frac{b}{\pi} \int_{-1}^1 \phi(s) \frac{ds}{s-x} + \lambda \int_{-1}^1 k(x, s) \phi(s) ds = f(x), \quad |x| < 1, \quad (9.7.14)$$

for which, by using the orthogonality properties of the Jacobi polynomials, Erdogan, Gupta and Cook (1973) derive an infinite system of linear algebraic equations

$$\phi(x) = \sum_{n=0}^{\infty} c_n w(x) P_n^{(\alpha, \beta)}(x), \quad (9.7.15)$$

where $w(x) = (1-x)^\alpha (1+x)^\beta$ and $c_n, n = 0, 1, \dots$, are constants to be determined. Before substituting (9.7.15) into Eq (9.7.14), note that for the index $\kappa = (-1, 0, 1)$ we have (see Tricomi 1957, Szegő 1939)

$$\begin{aligned} \frac{1}{\pi} \int_{-1}^1 w(s) P_n^{(\alpha, \beta)}(s) \frac{ds}{s-x} &= \cot(\pi\alpha) w(x) P_n^{(\alpha, \beta)}(x) \\ &\quad - \frac{2^{\alpha+\beta} \Gamma(\alpha) \Gamma(n+\beta+1)}{\pi \Gamma(n+\alpha+\beta+1)} F\left(n+1, -n-\alpha-\beta; 1-\alpha; \frac{1-x}{2}\right), \\ -1 < x < 1, \quad \Re\{\alpha\} > -1, \quad \Re\{\alpha\} \neq 0, 1, \dots, \quad \Re\{\beta\} > -1, \\ \cot(\pi\alpha) &= \cot \pi \left[\frac{1}{2i\pi} \log \left(\frac{a-ib}{a+ib} \right) + N \right] = -\frac{a}{b}, \quad \alpha + \beta = -\kappa, \end{aligned} \quad (9.7.16)$$

and

$$P_{n-\kappa}^{(-\alpha, -\beta)}(x) = \frac{\Gamma(n - \kappa - \alpha + 1)}{\Gamma(1 - \alpha) \Gamma(n - \kappa + 1)} F\left(n+1, -n+\kappa; 1-\alpha; \frac{1-x}{2}\right). \quad (9.7.17)$$

Hence, combining (9.7.16) and (9.7.17), we get

$$\begin{aligned} a w(x) P_n^{(\alpha, \beta)}(x) + \frac{b}{\pi} \int_{-1}^1 w(s) P_n^{(\alpha, \beta)}(s) \frac{ds}{s-x} \\ = -2^{-\kappa} b \frac{\Gamma(\alpha) \Gamma(1-\alpha)}{\pi} P_{n-\kappa}^{(-\alpha, -\beta)}(x), \quad |x| < 1. \end{aligned} \quad (9.7.18)$$

Then, substituting (9.7.15) into Eq (9.7.14) and using (9.7.18), we obtain an infinite system of algebraic equations

$$\sum_{n=0}^{\infty} c_n \left[-\frac{2^{-\kappa} b}{\sin(\pi\alpha)} P_{n-\kappa}^{(-\alpha, -\beta)}(x) + h_n(x) \right] = f(x), \quad (9.7.19)$$

where

$$h_n(x) = \lambda \int_{-1}^1 w(s) P_n^{(\alpha, \beta)}(s) k(x, s) ds, \quad |x| < 1.$$

Now, we use the orthogonality relations

$$\int_{-1}^1 P_n^{(\alpha, \beta)}(s) P_m^{(\alpha, \beta)}(s) w(s) ds = \begin{cases} 0 & \text{if } n \neq m, \\ \theta_m^{(\alpha, \beta)} & \text{if } n = m, \end{cases}$$

for $m = 0, 1, 2, \dots$, where

$$\theta_m^{(\alpha, \beta)} = \frac{2^{\alpha+\beta+1}}{2m + \alpha + \beta + 1} \frac{\Gamma(m + \alpha + 1) \Gamma(m + \beta + 1)}{m! \Gamma(m + \alpha + \beta + 1)}, \quad m = 0, 1, 2, \dots,$$

and

$$\theta_0^{(\alpha, \beta)} = \int_{-1}^1 w(s) ds = \frac{2^{\alpha+\beta+1} \Gamma(\alpha + 1) \Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)}.$$

Then we truncate the series (9.7.19) to obtain

$$-\frac{2^{-\kappa} b}{\sin(\pi\alpha)} \theta_m(-\alpha, -\beta) c_{m+\kappa} + \sum_{n=0}^N d_{nm} c_n = F_m, \quad m = 0, 1, \dots, N, \quad (9.7.20)$$

where

$$\begin{aligned} d_{nm} &= \int_{-1}^1 P_m^{(-\alpha, -\beta)}(x) w(-\alpha, -\beta, x) h_n(x) dx, \\ F_m &= \int_{-1}^1 P_m^{(-\alpha, -\beta)}(x) w(-\alpha, -\beta, x) f(x) dx, \\ w(-\alpha, -\beta, x) &= (1-x)^{-\alpha} (1+x)^{-\beta} = w^{-1}(x). \end{aligned} \quad (9.7.21)$$

There are three cases to consider.

CASE 1. $\kappa = -1$: Note that the first term of the series (9.7.19) is equal to a constant multiplied by $c_0 P_1^{(-\alpha, -\beta)}(x)$. Hence, in solving Eq (9.7.14) we can take $c_{-1} = 0$. Also, since $P_0^{(-\alpha, -\beta)}(x) = 1$, it can be seen from Eqs (9.7.20) and (9.7.21) that the first equation obtained from (9.7.20) for $m = 0$ is equivalent to the consistency condition

$$\int_{-1}^1 \left[f(x) - \int_{-1}^1 k(x, s) \phi(s) ds \right] \frac{ds}{w(s)} = 0.$$

Thus, Eqs (9.7.20) give $(N + 1)$ linear equations to compute the unknown constants c_0, \dots, c_N .

CASE 2. $\kappa = 0$: This case does not need any additional conditions, and Eqs (9.7.20) give the unique solution for c_0, \dots, c_N .

CASE 3. $\kappa = 1$: In this case there are $(N + 2)$ unknown constants c_0, \dots, c_{N+1} but only $(N + 1)$ equations given by (9.7.20). Thus, we need one more equation, which is provided by the equilibrium or compatibility condition $\int_{-1}^1 \phi(s) ds = A$, which, after its substitution into (9.7.15) and using the orthogonality condition, reduces to

$$c_0 \theta_0(\alpha, \beta) = A.$$

Then Eqs (9.7.20) together with this condition are solved to compute the $(N + 2)$ constants c_0, \dots, c_{N+1} .

9.8. Canonical Equation

The CSK1 of the form (9.6.2) on the interval $[-1, 1]$ is given by

$$\frac{1}{\pi} \oint_{-1}^1 \frac{\phi(s) ds}{s - x} + \lambda \int_{-1}^1 k(x, s) \phi(s) ds = f(x), \quad |x| < 1. \quad (9.8.1)$$

If $\lambda = 0$, we obtain the so-called canonical equation

$$\frac{1}{\pi} \oint_{-1}^1 \frac{\phi(s) ds}{s - x} = f(x), \quad |x| < 1, \quad (9.8.2)$$

which has a bounded solution iff

$$\frac{1}{\pi} \oint_{-1}^1 \frac{f(x) dx}{\sqrt{1 - x^2}} = 0. \quad (9.8.3)$$

If Eq (9.8.2) has bounded solution, then

$$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} \left\{ f(x) - \lambda \int_{-1}^1 k(x,s) \phi(s) ds \right\} dx = 0.$$

Since this equation contains $\phi(s)$, it cannot be used to check whether the necessity of the condition (9.8.3) is met unless $\int_{-1}^1 \frac{k(x,s)}{\sqrt{1-x^2}} dx = 0$ for almost all s . But this is obviously the case when $k(x,s)$ is an odd function of x .

The collocation method given above to compute a bounded solution of Eq (9.8.2) consists of the following steps:

1. Set $\phi(x) = \sqrt{1-x^2} g(x)$;
2. Replace the integrals by the Gaussian quadrature using the zeros of $U_n(x)$;
3. Generate the system of linear algebraic equations at the zeros of $T_{n+1}(x)$; and
4. Solve this system, which contains $(n+1)$ equations in n unknowns; thus ignore one equation.

Jen and Srivastav (1983, p. 626) observe that “in practice the most harmless point to neglect would be the one closest to $x = 0$.” Note that in steps 2 and 3 we use the nodes and Nyström points, given by

$$\text{Nodes:} \quad s_j = \cos \left(\frac{2j-1}{2n} \pi \right), \quad j = 1, \dots, n,$$

$$\text{Nyström points:} \quad x_i = \cos \left(\frac{i\pi}{n} \right), \quad i = 1, 2, \dots, n-1,$$

and the quadrature given by

$$\int_{-1}^1 \frac{\sqrt{1-s^2} g(s) ds}{s_j - x_i} = \frac{1}{2n+2} \sum_{j=1}^{2n+1} \frac{(1-s_j^2) g(s_j)}{s_j - x_i}. \quad (9.8.4)$$

Also, by a change of variable it is easy to verify that in the equation

$$\int_{-1}^1 \frac{\sqrt{1-s^2} g(s) ds}{s_j - x_i} = f(x), \quad |x| < 1, \quad (9.8.5)$$

$g(s)$ is an odd function of s if $f(x)$ is even, and $g(s)$ is an even function of s if $f(x)$ is odd. Hence, to solve Eq (9.8.2), first we split it into its ‘odd’ and ‘even’ parts, and then combine the regular part of Eq (9.8.2) with $f(x)$. Now, we consider the following two cases:

CASE 1. If $f(x)$ is odd and $g(s)$ is even, then a bounded solution always exists because the condition (9.8.3) is automatically satisfied. By using Gauss-Chebyshev rule (§3.2.7), Eq (9.8.5) reduces to

$$\frac{1}{2n+1} \sum_{j=1}^n \frac{(1-s_j^2) g(s_j) ds}{s_j - x_i} = f(x_i), \quad i = 1, \dots, 2n+1,$$

which, by using symmetry, can be written as

$$\frac{2}{2n+1} x_i^2 \sum_{j=1}^n \frac{(1-s_j^2) g(s_j) ds}{s_j^2 - x_i^2} = x_i f(x_i), \quad i = 1, \dots, n+1.$$

The equation corresponding to $i = n+1$ is automatically satisfied since $x_{n+1} = 0$. Hence, there are n equations in n unknowns $g(s_j)$, and the system is normal.

CASE 2. If $g(s)$ is odd, $f(x)$ is even and the condition (9.8.3) is satisfied, where the discrete form of this condition is $\sum_{i=1}^{2n+2} f(x_i) = 0$, which, since $f(x)$ is even and the distribution of the points x_i are symmetric, reduces to

$$\sum_{i=1}^{n+1} f(x_i) = 0, \quad (9.8.6)$$

then formula (9.8.4) yields the following system of linear algebraic equations:

$$\frac{1}{2n+2} \sum_{j=1}^n \frac{(1-s_j^2) g(s_j) ds}{s_j - x_i} = f(x_i), \quad i = 1, \dots, 2n+2. \quad (9.8.7)$$

This system is overdetermined but consistent (see [Jen and Srivastav 1983, p.629](#)). Notice that $s_{n+1} = 0$, and for continuous g we have $g(s_{n+1}) = 0$. Hence, the system (9.8.7) reduces to

$$\frac{1}{n+1} \sum_{j=1}^n \frac{s_j (1-s_j^2) g(s_j) ds}{s_j^2 - x_i^2} = f(x_i), \quad i = 1, \dots, n+1, \quad (9.8.8)$$

which has $n+1$ equations and n unknowns $g(s_j)$. This system can be written in matrix form as

$$\mathbf{A} \mathbf{g} = \mathbf{f}, \quad (9.8.9)$$

where $\mathbf{A} = (a_{i,j})$ is an $(n+1) \times n$ matrix with its (i,j) -th element given by

$$a_{i,j} = \frac{1}{n+1} \frac{s_j^2 (1-s_j^2)}{s_j^2 - x_i^2},$$

$\mathbf{g} = \{g_j\}$ is an $n \times 1$ vector with the j -th element $\frac{g(s_j)}{s_j}$, and $\mathbf{f} = \{f_i\}$ is an $(n+1) \times 1$ vector with the i -th element $f(x_i)$.

Now, a least squares solution of system (9.8.9) is obtained as follows: Introduce a 'phantom' variable $g(s_{n+1})$ that satisfies

$$\frac{1}{n+1} \sum_{j=1}^n \frac{s_j^2 (1-s_j^2) g(s_j) / s_j ds}{s_j^2 - x_i^2} + g(s_{n+1}) = f(x_i), \quad i = 1, \dots, n+1, \quad (9.8.10)$$

and consider the system

$$(\mathbf{A} \mathbf{e}) \tilde{\mathbf{g}} = \mathbf{f}, \quad (9.8.11)$$

where $\mathbf{e} = [1, 1, \dots, 1]^t$, and $\tilde{\mathbf{g}}$ is the vector \mathbf{g} augmented by the element $g(s_{n+1})$; thus, $\tilde{\mathbf{g}}$ is an $(n+1) \times 1$ vector. By using the identity $\sum_{j=1}^n (s_j^2 - x_i^2)^{-1} = 0$, for $i = 1, \dots, n-1$, where s_j are the zeros of the polynomial $T_{2n}(x)$ and x_i the zeros of the polynomial $U_{2n-1}(x)$, the columns of the coefficient matrix in (9.8.11) form an orthogonal basis in \mathcal{R}^{n+1} . The condition (9.8.6) implies that the vector \mathbf{f} is orthogonal to \mathbf{e} , i.e., $g(s_{n+1}) = 0$. Assuming that f satisfies the condition (9.8.3) but not (9.8.6), we find that the least-squares solution $\mathbf{g}^* = \{g_j^*\}$, $j = 1, \dots, n$, of the system (9.8.9) satisfies the system

$$\mathbf{A}^T \mathbf{A} \mathbf{g}^* = \mathbf{A}^T \mathbf{f}, \quad (9.8.12)$$

which is a normal system. Since the columns of \mathbf{A} are mutually orthogonal, we find that

$$g_j^* = \frac{1}{n+1} \sum_{i=1}^{n+1} \frac{f(x_i)}{s_j^2 - x_i^2}, \quad j = 1, \dots, n. \quad (9.8.13)$$

Note that the least-squares solution \mathbf{g}^* coincides with the phantom solution $\tilde{\mathbf{g}}$ in the sense that $\tilde{g}_j = g_j^*$ for $j = 1, \dots, n$, and $\tilde{g}_{n+1} = \frac{1}{n+1} \sum_{i=1}^{n+1} f(x_i)$. The quantity

$d = \frac{1}{n+1} \sum_{i=1}^{n+1} f(x_i)$, which defines the accuracy of the Gaussian quadrature, can be used as a *measure of inconsistency*. We consider the case where d differs significantly from zero for moderately large n , and solve the overdetermined system (9.8.9) by deleting one row from the matrix \mathbf{A} . The question is, which row should be deleted. Suppose that $\mathbf{g}^{(p)}$ is the solution vector of the system

$$\mathbf{A}^{(p)} \mathbf{g}^{(p)} = \mathbf{f}^{(p)}, \quad (9.8.14)$$

where $\mathbf{A}^{(p)}$ and $\mathbf{f}^{(p)}$ are obtained from the original system (9.8.9) by deleting the p -th row. Define an $n \times 1$ vector $\boldsymbol{\epsilon}^{(p)}$ by $\boldsymbol{\epsilon}^{(p)} = \mathbf{g}^* - \mathbf{g}^{(p)}$, and an $n \times 1$ vector \mathbf{d} by d_j , $j = 1, \dots, n$. Then $\boldsymbol{\epsilon}^{(p)}$ satisfies the system

$$\mathbf{A}^{(p)} \boldsymbol{\epsilon}^{(p)} = \mathbf{d}^{(p)}. \quad (9.8.15)$$

Instead of solving (9.8.15) directly, we use the properties of the matrix \mathbf{A} to compute $\boldsymbol{\epsilon}^{(p)}$ as follows: Define an $(n+1) \times 1$ vector \mathbf{d}^* by $d_j^* = d$, $j = 1, \dots, n+1$, $j \neq p$, and $d_p^* = -nd$, and consider the augmented system

$$(\mathbf{A} \mathbf{e}) \boldsymbol{\epsilon} = \mathbf{d}^*, \quad (9.8.16)$$

where ϵ is augmented by a ‘phantom’ element ϵ_{n+1} . Since the right side of vector \mathbf{d}^* satisfies the consistency condition (9.8.6), we find by using the orthogonality properties of the coefficient matrix that

$$\epsilon_j^{(p)} = -d \frac{s_j}{s_j^2 - x_i^2}, \quad j = 1, \dots, n; \quad p = 1, \dots, n+1, \quad (9.8.17)$$

determines the discrepancy in the j -th element of the solution vector caused by deleting the p -th row of the system. The error in $g(s)$ is, therefore, determined by

$$\epsilon_j^{*(p)} = -d \frac{s_j \sqrt{1 - s_j^2}}{s_j^2 - x_i^2}. \quad (9.8.18)$$

Jen and Srivastav (1983) compute $\epsilon_j^{*(p)}$ for $n = 20$, $d = 1$, and $p = 1, 7, 14, 18, 21$, and observe that the error is maximum near the deleted row. They advise that the choice of the row to be deleted must depend on the quantity of interest in the problem; e.g., in crack problems if the stress near the endpoints needs be computed, then choose the deleted value of s_j which is closest to zero. But if we seek the entire crack profile and maximum crack displacement, then choose the deleted value s_j which is farthest from zero.

EXAMPLE 9.8.1. (Jen and Srivastav 1983) Consider the canonical equation

$$\int_{-1}^1 \frac{g(s) \sqrt{1 - s^2}}{s - x} ds = \frac{1 - a^2}{1 - 2ax + a^2} - 1, \quad |x| < 1,$$

with $a^2 = 0.95$. Let $f_0(x)$ denote the even part of the right side $f(x)$. Then $\int_{-1}^1 \frac{f_0(x)}{\sqrt{1 - x^2}} dx = 0$, and the compatibility condition is satisfied. Thus, the exact

solution is given by the odd part (case 2), i.e., $g(x) = -\frac{2a}{1 - 2ax + a^2}$. Tables 9.8.1(a) and 9.8.1(b) give the numerical solutions obtained by Jen and Srivastav (1983) with $n = 20$ and $n = 60$, respectively, and show the deleted row of the overdetermined system. Note that the discrepancy between the exact and computed values depends only on the value of d chosen, and not on the solution itself. Columns 2 and 3 give the exact values and the values obtained by the least-squares method, respectively, and the last three columns give the values of $\epsilon^*(s)$ for different values of p .

9.9. Finite-Part Singular Equations

We apply the product integration method to equations of the form

$$\phi(x) = f(x) + \oint_a^b \frac{\hat{k}(x, s)}{(x - s)^\alpha} \phi(s) ds, \quad a < x < b, \quad \alpha > 1, \quad (9.9.1)$$

where the integration is in the finite-part or Hadamard sense (see §5.4.3; also [Davis and Rabinowitz](#) 1984, pp. 11–13). Equations of the above form are strongly singular and are encountered in fracture mechanics, gas radiation, and fluid flow ([Kaya and Erdogan](#) 1987).

Table 9.8.1(a). For $n = 20$, $d = -0.2079$

s	$g(s)$	$\tilde{g}(s)$	$p = 21$	$p = 10$	$p = 1$
0.9972	-11.9377	-9.4564	-0.0156	-0.0369	3.7
0.9749	-4.3238	-3.4251	-0.0475	-0.1200	0.9372
0.9309	-2.5355	-2.0084	-0.0817	-0.2421	0.5352
0.8660	-1.7275	-1.3684	-0.1202	-0.5129	0.3620
0.7818	-1.2518	-0.9916	-0.1661	-2.7579	0.2247
0.6801	-0.9267	-0.7341	-0.2247	0.9263	0.1661
0.5633	-0.6811	-0.5296	-0.3062	0.3762	0.1202
0.4339	-0.4812	-0.3812	-0.4349	0.2104	0.0817
0.2948	-0.3082	-0.2442	-0.6849	0.1201	0.0475
0.1490	-0.1506	-0.1193	-1.4717	0.0555	0.0156
0.0	0.0	0.0	—	—	—

Table 9.8.1(b). For $n = 60$, $d = -0.0038$

s	$g(s)$	$\tilde{g}(s)$	$p = 61$	$p = 30$	$p = 1$
0.9937	-19.4869	-19.4121	-0.0001	-0.0002	0.1984
0.9838	-5.3774	-5.3568	-0.0007	-0.0015	0.0211
0.9449	-2.8574	-2.8464	-0.0013	-0.0032	0.0110
0.8827	-1.8726	-1.8654	-0.0020	-0.0063	0.0072
0.7998	-1.3302	-1.3251	-0.0029	-0.0161	0.0051
0.6979	-0.9733	-0.9696	-0.0039	0.0496	0.0037
0.5794	-0.7102	-0.7075	-0.0054	0.0095	0.0017
0.4471	-0.4994	-0.4975	-0.0077	0.0047	0.0019
0.3041	-0.3190	-0.3178	-0.0120	0.0025	0.0012
0.1539	-0.1556	-0.1550	-0.0248	0.0012	0.0006
0.0	0.0	-0.0038	—	—	— ■

As before, we partition the interval $[a, b]$ into n parts by $a = s_1 < s_2 < \dots < s_{n+1} = b$. On the subinterval $[s_j, s_{j+2}]$ we interpolate $\hat{k}(x, s)\phi(s)$ by a quadratic polynomial. Then we use Nyström method by taking $x = s_i$, $i = 1, \dots, n+1$, and approximate the integral by a sum of the form $\sum_{j=1}^n w_{ij}(x)k(s_i, s_j)\tilde{\phi}(s_j)$, as in

(9.3.2), where in this case the weights w_{ij} are given by (see [Bertram and Ruehr 1992](#))

$$\begin{aligned} w_{i0} &= 2n - \frac{1}{x} + n^2 \left(x - \frac{3}{2n} \right) \ln \left| \frac{\frac{2}{n} - x}{x} \right|, \\ w_{i,2j} &= 4n + 3n \ln \left| \frac{j}{n} - x \right| + n^2 \left(x - \frac{2j+3}{n} \right) \\ &\quad - n^2 \left(x - \frac{2j-3}{2n} \right) \ln \left| \frac{j-2}{n} - x \right|, \quad j = 1, \dots, n-1, \\ w_{i,2j+1} &= -4n + 2n^2 \left(x - \frac{j}{n} \right) \ln \left| \frac{x - \frac{j-1}{n}}{x - \frac{j+1}{n}} \right|, \quad j = 1, \dots, n-1, \\ w_{i,n} &= 2n + \frac{1}{x-1} + n^2 \left(x - \frac{2n-3}{2n} \right) \ln \left| \frac{\frac{1-x}{n-2}}{\frac{n-2}{n} - x} \right|. \end{aligned}$$

This leads to a linear $(2n-1) \times (2n-1)$ system that can be solved to yield approximate values $\tilde{\phi}$ at s_2, \dots, s_n .

EXAMPLE 9.9.1. ([Bertram and Ruehr 1992](#)) We shall consider the case when $\alpha = 2$. Then $p(x, s) = \frac{\hat{k}(x, s)}{(x-s)^2}$, and with $a = 0, b = 1$ Eq (9.9.1) becomes

$$\phi(x) = f(x) + \oint_0^1 \frac{\phi(s)}{(x-s)^2} ds. \quad (9.9.2)$$

[Table 5.4.5](#) gives the Hadamard transform $H_2[\phi]$ defined by

$$H_2[\phi] = \oint_0^1 \frac{\phi(s)}{(x-s)^2} ds \quad (9.9.3)$$

for functions $\phi(x)$ that exhibit different types of singularities, as in (1)–(3) where $\phi(x) = x^\beta(1-x)^\gamma$ for rational β and γ ; in (4) internal (jump) singularities; in (5)–(6) singularities (jump) in the first derivative, and those in (7) in the second derivative; we have also included a smooth function $\phi(x) = \sin \pi x$ in (8). Note that in the finite-part (Hadamard) sense the infinite values of poles and logarithms should be discarded in the second column of this table, and according to a convention in finite-part interpretation we take $\ln(0) = 0$.

Let $f = \phi - H_2[\phi]$. Then we can determine the error for any approximate solution $\tilde{\phi}$. [Bertram and Ruehr \(1992\)](#) have postulated that for sufficiently large n the error at the n -th approximation is given by

$$e_n = |\phi(x) - \tilde{\phi}_n(x)| = \frac{A}{n^p} + \frac{B}{n^{p+1}} + O\left(\frac{1}{n^{p+2}}\right), \quad (9.9.4)$$

where n is the number of subintervals of $[a, b]$ used in the above method. ■

For examples of Hadamard's finite-part integrals, see §5.4.3 and §5.4.4.

9.10. Integral Equations over a Contour

Linear equations FK1 are not always in the form (9.1.1). Sometimes the integral in the equation appears as a contour integral where the free variable lies on a contour C . However, such equations can be transformed to the form (9.1.1) after parametrizing the contour C by the arc length measured from a fixed point on C . If C is a closed contour, the integrand $k(x, s)\phi(s)$ becomes periodic with a period equal to the length of C . Then the trapezoidal rule yields high-order local truncation errors if $k(x, s)$ and $\phi(x)$ are smooth.

EXAMPLE 9.10.1. Consider an FK1 with a weakly singular kernel

$$\int_C \ln |z - \zeta| \phi(\zeta) |d\zeta| = f(z), \quad z \in C,$$

where z and ζ are complex and the contour C is a circle with center at $z = 0$ and radius r . Such equations arise in conformal mappings (see [Kythe 1998](#)). Take a point P on the contour C as $\zeta = re^{i\theta}$, where θ is the angle that the radius vector OP makes with the real axis. Thus, $|d\zeta| = r |d\theta| = r d\theta$. Let $z = re^{i\delta}$, where r is fixed and δ is the free variable, $0 \leq \delta \leq 2\pi$, be a point on C . Then

$$\int_C \ln |z - \zeta| \phi(\zeta) |d\zeta| = r \int_0^{2\pi} \ln |e^{i\delta} - e^{i\theta}| \phi(re^{i\theta}) d\theta = f(re^{i\delta}).$$

This example, though an FK1, illustrates the formulation on integral equations, which generally involves contour integration. ■

EXAMPLE 9.10.2. Consider integral equations that involve integration on a contour C (closed or unclosed), which have the form

$$\phi(z) - \lambda \int_C k(z, \sigma) \phi(\sigma) d\sigma = f(z). \quad (9.10.1)$$

A method for solving this equation consists of choosing points s_0, s_1, \dots, s_n on C (note that $s_n = s_0$ if C is closed) and denoting the arc joining the points s_j, s_{j+1} by C_j , with length $h_j = |s_{j+1} - s_j|$. Then Eq (9.10.1) in the case of a closed contour C can be written as

$$\phi(z) - \lambda \sum_{j=0}^{n-1} \int_{C_j} k(z, \sigma) \phi(\sigma) d\sigma = f(z). \quad (9.10.2)$$

Let z_j be a point on C_j . Then we seek to determine the values $\tilde{\phi}(z_m)$, $m = 0, 1, \dots, n$, such that

$$\tilde{\phi}(z_m) - \lambda \sum_{j=0}^{n-1} \tilde{\phi}(z_j) \int_{C_j} k(z_m, \sigma) d\sigma = f(z_m). \quad (9.10.3)$$

But it may be difficult to compute $\int_{C_j} k(z_m, \sigma) d\sigma$, even when C is a line segment $[a, b]$. Therefore, if $m \neq j$, we will apply the quadrature rule

$$\int_{C_j} k(z_m, \sigma) d\sigma = \sum_{i=0}^{n_j} w_{ij} k(z_m, \sigma_{ij}) \quad (9.10.4)$$

to compute the integral on the left side over those points of C_j that do not contain the point z_m (in this case the integrand remains bounded). For the case when $m = j$ we need some method to avoid unbounded quantities (singularities). One such method to solve Symm's equation (Symm 1966) involves an approximate solution for the integral $\int_{C_j} \log |z_m - \sigma| d\sigma$ by using Simpson's rule:

$$\begin{aligned} & \int_{C_j} \log |z_m - \sigma| |d\sigma| \\ &= \begin{cases} \frac{h_j}{6} \left\{ \log |z_m - s_j| + 4 \log |z_m - z_j| + \log |z_m - s_{j+1}| \right\} & \text{if } m \neq j, \\ |z_j - s_j| \left\{ \log |z_j - s_j| - 1 \right\} \\ \quad + \log |z_j - z_{j+1}| \left\{ \log |z_j - s_{j+1}| - 1 \right\} & \text{if } m = j, \end{cases} \end{aligned} \quad (9.10.5)$$

where z_j is the middle point of C_j . For more information on Symm's equation, and other equations of conformal mappings including Lichtenstein's, Gershgorin's, Carrier's, Bannin's, Waeschawski-Stiefel's, Theodorsen's, Arbenz', and Mikhlin's equation, see [Trefethen](#) (1986) and [Kythe](#) (1998). ■

9.5.1. Boundary Element Method. There are many books on this subject; for example, the book by [Kythe](#) (1995) on this subject is a good source for the description of the method as well as computer codes. A summary of this method together with computer codes is available in the directory `bem.pdf` on the CD-R.

A

Quadrature Tables

Various tables used in quadrature rules are presented.

Table A.1. Cotesian Numbers, Tabulated for $k \leq n/2$, $n = 1(1)11$.

n	C_0^n	C_1^N	C_2^n	C_3^n	C_4^n	C_5^n
1	$\frac{1}{2}$					
2	$\frac{1}{6}$	$\frac{4}{6}$				
3	$\frac{1}{8}$	$\frac{3}{8}$				
4	$\frac{7}{90}$	$\frac{32}{90}$	$\frac{12}{90}$			
5	$\frac{19}{288}$	$\frac{75}{288}$	$\frac{50}{288}$			
6	$\frac{41}{840}$	$\frac{216}{840}$	$\frac{27}{840}$	$\frac{272}{840}$		
7	$\frac{751}{17280}$	$\frac{3577}{17280}$	$-\frac{928}{17280}$	$\frac{10496}{17280}$		
8	$\frac{989}{28350}$	$\frac{5888}{28350}$	$\frac{1323}{28350}$	$\frac{2989}{28350}$	$-\frac{4540}{28350}$	
9	$\frac{2857}{89600}$	$\frac{315741}{89600}$	$\frac{1080}{89600}$	$\frac{19344}{89600}$	$\frac{5778}{89600}$	
10	$\frac{16067}{598752}$	$\frac{106300}{598752}$	$-\frac{48525}{598752}$	$\frac{272400}{598752}$	$-\frac{260550}{598752}$	$\frac{427368}{598752}$
11	$\frac{2171465}{87091200}$	$\frac{13486539}{87091200}$	$-\frac{3237113}{87091200}$	$\frac{25226685}{87091200}$	$-\frac{9595542}{87091200}$	$\frac{15493566}{87091200}$

Table A.2. Weights for a Single Trapezoidal Rule and Repeated Simpson’s Rule.*

$m \setminus j$	0	1	2	3	4	5
1	$h/2$	$h/2$				
2	$h/3$	$4h/3$	$h/3$			
3	$h/2$	$5h/6$	$4h/3$	$h/3$		
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
5	$h/2$	$5h/6$	$4h/3$	$2h/3$	$4h/3$	$h/3$

Table A.3. Weights for Repeated Simpson’s Rule and a Single Trapezoidal Rule.

$m \setminus j$	0	1	2	3	4	5
1	$h/2$	$h/2$				
2	$h/3$	$4h/3$	$h/3$			
3	$h/3$	$4h/3$	$5h/6$	$h/2$		
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
5	$h/3$	$4h/3$	$2h/3$	$4h/3$	$5h/6$	$h/2$

Table A.4. Weights for a Single 3/8-Rule and Repeated Simpson’s Rule.

$m \setminus j$	0	1	2	3	4	5	6
1	$h/2$	$h/2$					
2	$h/3$	$4h/3$	$h/3$				
3	$3h/8$	$9h/8$	$9h/8$	$3h/8$			
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$		
5	$3h/8$	$9h/8$	$9h/8$	$17h/24$	$4h/3$	$h/3$	
6	$h/3$	$4h/3$	$2h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$

* Trapezoidal rule is used for integral \int_0^h and Simpson’s rule for the remainder of the integral.

Table A.5. Weights for Repeated Simpson's Rule and a Single 3/8-Rule.

$m \setminus j$	0	1	2	3	4	5	6	7
1	$h/2$	$h/2$						
2	$h/3$	$4h/3$	$h/3$					
3	$3h/8$	$9h/8$	$9h/8$	$3h/8$				
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$			
5*	$h/3$	$4h/3$	$17h/24$	$9h/8$	$9h/8$	$3h/8$		
6	$h/3$	$4h/3$	$2h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
7*	$h/3$	$4h/3$	$2h/3$	$4h/3$	$17h/24$	$9h/8$	$9h/8$	$3h/8$

The asterisk (*) indicates values that differ from corresponding values in [Table A.1](#). The above table has practical advantages over Table A.1.

Table A.6. Gauss-Legendre Quadrature.

$$w(x) = 1, \quad \int_{-1}^1 f(x) dx \approx \sum_{k=1}^n w_k f(x_k).$$

n	Nodes $\pm x_k$	Weights w_k
2	0.57735 02691 89626	1.
3	0. 0.77459 66692 41483	0.88888 88888 88889 0.55555 55555 55556
4	0.33998 10435 84856 0.86113 63115 94053	0.65214 51548 62546 0.34785 48451 37454
5	0. 0.53846 93101 05683 0.90617 98459 38664	0.56888 88888 88889 0.47862 86704 99366 0.23692 68850 56189
6	0.23861 91860 83197 0.66120 93864 66265 0.93246 95142 03152	0.46791 39345 72691 0.36076 15730 48139 0.17132 44923 79170
7	0. 0.40484 51513 77397 0.74153 11855 00394 0.94910 79123 42759	0.41795 91836 73469 0.38183 00505 05119 0.27970 53914 89277 0.12948 49661 68870
8	0.18343 46424 95650 0.52553 24099 16329 0.79666 64774 13627 0.96028 98564 97536	0.36268 37833 78362 0.31370 66458 77887 0.22238 10344 53374 0.10122 85362 90376

Continued

Table A.6. Gauss-Legendre Quadrature, Continued.

$$w(x) = 1, \quad \int_{-1}^1 f(x) \, dx \approx \sum_{k=1}^n w_k \, f(x_k).$$

<i>n</i>	Nodes $\pm x_k$	Weights w_k
9	0.	0.33023 93550 01260
	0.32425 34234 03809	0.31234 70770 40003
	0.61337 14327 00590	0.26061 06964 02935
	0.83603 11073 26636	0.18064 81606 94857
	0.96816 02395 07626	0.08127 43883 61574
10	0.14887 43389 81631	0.29552 42247 14753
	0.43389 53941 29247	0.26926 67193 09996
	0.67940 95682 99024	0.21908 63625 15982
	0.86506 33666 88985	0.14945 13491 50581
	0.97390 65285 17172	0.06667 13443 08688
16	0.09501 25098 37637	0.18945 06104 55068
	0.28160 35507 79259	0.18260 34150 44924
	0.45801 67776 57227	0.16915 65193 95003
	0.61787 62444 02644	0.14959 59888 16577
	0.75540 44083 55003	0.12462 89712 55534
	0.86563 12023 87832	0.09515 85116 82493
	0.94457 50230 73233	0.06225 35239 38648

Table A.7. Gauss-Laguerre Quadrature.

$$\int_0^1 f(x) \ln x \, dx \approx \sum_{k=1}^n w_k f(x_k).$$

n	Nodes $\pm x_k$	Weights w_k
2	0.58578 64376 27	8.53553 390593(−01)
	3.41421 35623 73	1.46446 609407(−01)
4	0.41577 45567 83	7.11093 009929(−01)
	2.29428 03602 79	2.78517 733569(−01)
	6.28994 50829 37	1.03892 565016(−02)
8	0.32254 76896 19	6.03154 104342(−01)
	1.74576 11011 58	3.57418 692438(−01)
	4.53662 02969 21	3.88879 085150(−02)
	9.39507 09123 01	5.39294 705561(−04)
10	0.26356 03197 18	5.21755 610583(−01)
	1.41340 30591 07	3.98666 811083(−01)
	3.59642 57710 41	7.59424 496817(−02)
	7.08581 00058 59	3.61175 867992(−03)
	12.64080 08442 76	2.33699 723858(−05)
	0.22284 66041 79	4.58964 673950(−01)
	1.18893 21016 73	4.17000 830772(−01)
	2.99273 63260 59	1.13373 382074(−01)
	5.77514 35691 05	1.03991 974531(−02)
	9.83746 74183 83	2.61017 202815(−04)
	15.98287 39806 02	8.98547 906430(−07)

Table A.8. Gauss-Hermite Quadrature.

$$w(x) = e^{-x^2}, \quad \int_{-\infty}^{\infty} e^{-x^2} f(x) dx \approx \sum_{k=1}^n w_k f(x_k).$$

<i>n</i>	Nodes $\pm x_k$	Weights w_k	$w_k e^{x_k^2}$
2	0.70710 67811 86548	8.86226 92545 28(−01)	1.46114 11826 611
3	0. 1.22474 48713 91589	1.18163 59006 04(+00) 2.95408 97515 09(−01)	1.18163 59006 037 1.32393 11752 136
4	0.52464 76232 75290 1.65068 01238 85785	8.04914 09000 55(−01) 8.13128 35447 25(−02)	1.05996 44828 950 1.24022 58176 958
5	0. 0.95857 24646 13819 2.02018 28704 56086	9.45308 72048 29(−01) 3.93619 32315 22(−01) 1.99532 42059 05(−02)	0.94530 87204 829 0.98658 09967 514 1.18148 86255 360
6	0.43607 74119 27617 1.33584 90740 13697 2.35060 49736 74492	7.24629 59522 44(−01) 1.57067 32032 29(−01) 4.53000 99055 09(−03)	0.87640 13344 362 0.93558 05576 312 1.13690 83326 745
7	0. 0.81628 78828 58965 1.67355 16287 67471 2.65196 13568 35233	8.10264 61755 68(−01) 4.25607 25261 01(−01) 5.45155 82819 13(−02) 9.71781 24509 95(−04)	0.81026 46115 568 0.82868 73032 836 0.89718 46002 252 1.10133 07296 103
8	0.38118 69902 07322 1.15719 37124 46780 1.98165 67566 95843 2.93063 74202 57244	6.61147 01255 82(−01) 2.07802 32581 49(−01) 1.70779 83007 41(−02) 1.99604 07221 14(−04)	0.76454 41286 517 0.79289 00483 864 0.86675 26065 634 1.07193 01442 480
9	0. 0.72355 10187 52838 1.46855 32892 16668 2.26658 05845 31843 3.19099 32017 81528	7.20235 21560 61(−01) 4.32651 55900 26(−01) 8.84745 27394 38(−02) 4.94362 42755 37(−03) 3.96069 77263 26(−05)	0.72023 52156 061 0.73030 24527 451 0.76460 81250 946 0.84175 27014 787 1.04700 35809 767
10	0.34290 13272 23705 1.03661 08297 89514 1.75668 36492 99882 2.53273 16742 32790 3.43615 91188 37738	6.10862 63373 53(−01) 2.40138 61108 23(−01) 3.38743 94455 48(−02) 1.34364 57467 81(−03) 7.64043 28552 33(−06)	0.68708 18539 513 0.70329 63231 049 0.74144 19319 436 0.82066 61264 048 1.02545 16913 657

Continued

Table A.8. Gauss-Hermite Quadrature, Continued.

n	Nodes $\pm x_k$	Weights w_k	$w_k e^{x_k}$
12	0.31424 03762 54359	5.70135 23626 25(−01)	0.62930 78743 695
	0.94778 83912 40164	2.60492 31026 42(−01)	0.63962 12320 203
	1.59768 26351 52605	5.16079 85615 88(−02)	0.66266 27732 669
	2.27950 70 <i>B</i> 05 01060	3.90539 05846 29(−03)	0.70522 03661 122
	3.02063 70251 20890	8.57368 70435 88(−05)	0.78664 39394 633
	3.88972 48 <i>i</i> 78 69782	2.65855 16843 56(−07)	0.98969 90470 923
16	0.27348 10461 3815	5.07929 47901 66(−01)	0.54737 52050 378
	0.82295 14491 4466	2.80647 45852 85(−01)	0.55244 19573 675
	1.38025 85391 9888	8.38100 41398 99(−02)	0.56321 78290 882
	1.95178 79909 1625	1.28803 11535 51(−02)	0.58124 72754 009
	2.54620 21578 4748	9.32284 00862 42(−04)	0.60973 69582 560
	3.17699 91619 7996	2.71186 00925 38(−05)	0.65575 56728 761
	3.86944 79048 6012	2.32098 08448 65(−07)	0.73824 56222 777
	4.68873 89393 0582	2.65480 74740 11(−10)	0.93687 44928 841

Table A.9. Gauss-Radau Quadrature.

$$\int_{-1}^1 f(x) \, dx \approx w_1 f(-1) + \sum_{k=2}^n w_k f(x_k), \quad -1 < \xi < 1, \text{ where each free node } x_k \text{ is the } k\text{-th root of } \frac{P_{n-1}(x) + P_n(x)}{[(2n-1)!]^3} f^{(2n-1)}(\xi), \, k = 2, \dots, n, \text{ and } x_1 = -1 \text{ and } w_1 = 2/n^2.$$

<i>n</i>	Nodes <i>x_k</i>	Weights <i>w_k</i>
3	0.28989 79485	1.02497 16523
	0.68989 79485	0.75280 61254
4	−0.57531 89235	0.65768 86399
	0.18106 62711	0.77638 69376
	0.82282 40809	0.44092 44223
5	−0.72048 02713	0.44620 78021
	−0.16718 08647	0.62365 30459
	0.44631 39727	0.56271 20302
	0.88579 16077	0.28742 71215
6	−0.80292 98284	0.31964 07532
	−0.39092 85467	0.48538 71884
	0.12405 03795	0.52092 67831
	0.60397 31642	0.41690 13343
	0.92038 02858	0.20158 83852
7	−0.85389 13426	0.23922 74892
	−0.53846 77240	0.38094 98736
	−0.11734 30375	0.44710 98290
	0.32603 06194	0.42740 37790
	0.70384 28006	0.31820 42314
	0.94136 71456	0.14898 84711
8	−0.88747 78789	0.18535 81548
	−0.63951 86165	0.30413 06206
	−0.29475 05657	0.37651 75453
	0.09430 72526	0.39157 21674
	0.46842 03544	0.34701 47956
	0.77064 18936	0.24964 79013
	0.95504 12271	0.11450 88147

Continued

Table A.9. Gauss-Radau Quadrature, Continued.

9	−0.01073 20894	0.14765 40190
	−0.71126 74859	0.24718 93782
	−0.42635 04857	0.31684 37756
	−0.09037 33696	0.34827 30027
	0.25613 56708	0.33769 39669
	0.57138 30412	0.28638 66903
	0.81735 27842	0.20055 32980
	0.96444 01697	0.09071 45049
10	−0.92748 43742	0.12029 66705
	−0.76384 20424	0.20427 01318
	−0.52564 60303	0.26819 48378
	−0.23623 44693	0.30585 92877
	0.07605 91978	0.31358 24572
	0.38066 48401	0.29061 01648
	0.64776 66976	0.23919 34317
	0.85122 52205	0.16437 60127
	0.97117 51807	0.07361 70054

Table A.10. Gauss-Lobatto Quadrature.

$$\int_{-1}^1 f(x) \, dx \approx w_1 f(-1) + w_n f(1) + \sum_{k=2}^n w_k f(x_k)$$

$$- \frac{n(n-1)3^{2n-1} [(n-2)!]^4}{(2n-1) [(2n-2)!]^3} f^{(2n-2)}(\xi), \quad -1 < \xi < 1, \text{ where}$$

$$x_k \text{ is the } (k-1)\text{-st root of } P'_{n-1}(x) \text{ and } w_k = \frac{2}{n(n-1)P_{n-1}(x_k))^2} \text{ for } k =$$

$$2, \dots, n-1; x_1 = -1, x_n = 1, \text{ and } w_1 = w_n = 2/(n(n-1)).$$

<i>n</i>	Nodes $\pm x_k$	Weights w_k
3	1.	0.33333 33333
	0.	1.33333 33333
4	1.	0.16666 66667
	0.44721 35954	0.83333 33333
5	1.	0.10000 000
	0.65465 36707	0.54444 44444
6	1.	0.06666 66667
	0.76505 53239	0.37847 49562
	0.28523 15164	0.55485 83770
7	1.	0.04761 90476
	0.83022 38962	0.27682 60473
	0.46884 87934	0.43174 53812
	0.	0.48761 90476
8	1.	0.03571 42857
	0.87174 01485	0.21070 42271
	0.59170 01814	0.34112 26924
	0.20929 92179	0.41245 87946
9	1.	0.02777 77778
	0.89975 79954	0.16549 53616
	0.67718 62795	0.27453 87126
	0.36311 74638	0.34642 85110
	0.	0.3715 192744
10	1.	0.022222222
	0.91953 39082	0.13330 59908
	0.73877 38651	0.22488 93420
	0.47792 49498	0.29204 26836
	0.16527 89577	0.32753 97612

Table A.11. Nodes of Equal-Weight Chebyshev Rule.

n	$\pm x_i$	n	$\pm x_i$	n	$\pm x_i$
2	0.57735 02692	5	0.83249 74870 0.37454 14096 0.00000 00000	7	0.88386 17008 0.52965 67753 0.32391 18105 0.00000 00000
3	0.70710 67812 0.00000 00000			9	0.91158 93077 0.60101 86554 0.52876 17831 0.16790 61842 0.00000 00000
		6	0.86624 68181 0.42251 86538 0.26663 54015		
4	0.79465 44723 0.18759 24741				

Table A.12. Gauss-Log Quadrature.

n	Nodes $\pm x_k$	Weights w_k
2	0.11200 88061 66976 18296 0.60227 69081 18738 10276	0.71853 93190 30384 44067 0.28146 06809 69615 55933
4	0.41448 48019 93832 20803(−01) 0.24527 49143 20602 25194 0.55616 54535 60275 83718 0.84898 23945 32985 17465	0.38346 40681 45135 12485 0.38687 53177 74762 62734 0.19043 51269 50142 41536 0.39225 48712 99598 32453(−01)
8	0.13320 24416 08924 65012(−01) 0.79750 42901 38949 38410(−01) 0.19787 10293 26188 05379 0.35415 39943 51909 41967 0.52945 85752 34917 27771 0.70181 45299 39099 96384 0.84937 93204 41106 67605 0.95332 64500 56359 78877	0.16441 66047 28002 88683 0.23752 56100 23306 02050 0.22684 19844 31919 12637 0.17575 40790 06070 24499 0.11292 40302 46759 05186 0.57872 21071 77820 72399(−01) 0.20979 07374 21329 78043(−01) 0.36864 07104 02761 90134(−02)

Continued

Table A.12. Gauss-Log Quadrature, Continued.

16	0.38978 34487 11591 59241(−02)	0.60791 71004 35912, 32851(−01)
	0.23028 94561 68732 39820(−01)	0.10291 56775 17582 14439
	0.58280 39830 62404 12348(−01)	0.12235 56620 46009 19356
	0.10867 83650 91054 03649	0.12756 92469 37015 98872
	0.17260 94549 09843 93776	0.12301 35746 00070 91542
	0.24793 70544 70578 49515	0.11184 72448 55485 72262
	0.33209 45491 29917 15598	0.96596 38515 21243 41253(−01)
	0.42218 39105 81948 60012	0.79356 66435 14731 38782(−01)
	0.51508 24733 81462 60348	0.61850 49458 19652 07095(−01)
	0.60755 61204 47728 72409	0.45435 24650 77266 68629(−01)
	0.69637 56532 28214 06116	0.31098 97475 15818 06409(−01)
	0.77843 25658 73265 40520	0.19459 76592 73608 42078(−01)
	0.85085 02697 15391 08323	0.10776 25496 32055 25646(−01)
	0.91108 68572 22271 90542	0.49725 42890 08764 17125(−02)
	0.95702 55717 03542 15759	0.16782 01110 05119 45150(−02)
	0.98704 78002 47984 47676	0.28235 37646 68436 32178(−03)

Table A.13. Gauss-Kronrod Quadrature Rule.

n	Nodes x_i	Weights w_i for $G_n(f)$	Weights W_i for $K_n(f)$
1	0.1127016653792582	0.0	0.2777777777777777
	0.5	1.0	0.4444444444444444
	0.8872983346207418	0.0	0.2777777777777777
2	0.0370899501137243	0.0	0.0989898989898989
	0.2113246854051871	0.5	0.2454545454545454
	0.5	0.0	0.3111111111111111
	0.7886751345948129	0.5	0.2454545454545454
	0.9629100498862757	0.0	0.0989898989898989
3	0.0197543656459899	0.0	0.0528281130132336
	0.1127016653792583	0.2777777777777777	0.1342440449341667
	0.2828781253265987	0.0	0.2006987073879811
	0.5	0.4444444444444444	0.2254582693292372
	0.7171218746734013	0.00	0.2006987073879811
	0.8872983346207417	0.2777777777777777	0.1342440449341667
	0.9802456843540101	0.0	0.0528281130132336
4	0.0117198746312134	0.0	0.0314886868827365
	0.0694318442029787	0.1739274225687269	0.0850268026678614
	0.1798568912518450	0.0	0.1333991702261422
	0.3300094782075719	0.3260725774312781	0.1634745948007258
	0.5	0.0	0.1732214909457258
	0.6699905217924281	0.3260725774312781	0.1634745948007258
	0.8201481087481550	0.0	0.1333991702261422
	0.9805681557970268	0.1739274225687269	0.0850268026678614
	0.9882801253687866	0.0	0.0314886868827365
5	0.0079573199525788	0.0000000000000000	0.0212910183755409
	0.0469100770306680	0.1184634425280945	0.0576166583112367
	0.1229166867145754	0.0	0.0934008982782463
	0.2307653449471585	0.2393143352496833	0.1205201696143238
	0.3601847934191084	0.0	0.1364249009562795
	0.5	0.2844444444444444	0.1414937089287456
	0.6398152065808916	0.0	0.1364249009562795
	0.7692346550528415	0.2393143352496833	0.1205201696143238
	0.8770833632854246	0.0	0.0934008982782463
	0.9530899229693320	0.1184634425280945	0.0576166583112367
	0.9992042680047421	0.0	0.0212910183755409

Table A.14. Patterson’s Quadrature Rule.
 $w(x) = 1, \quad \int_{-1}^1 f(x) \, dx \approx \sum_{k=1}^n w_k \, f(x_k).$

<i>n</i>	Nodes $\pm x_k$	Weights w_k
3	0.77459 66692 41483 37704 0.0	0.55555 55555 55555 555556 0.88888 88888 88888 888889
7	0.96049 12687 08020 28342 0.77459 66692 41483 37704 0.43424 37493 46802 55800 0.0	0.10465 62260 26467 265194 0.26848 80898 68333 440729 0.40139 74147 75962 222905 0.45091 65386 58474 142345
15	0.99383 19632 12755 02221 0.96049 12687 08020 28342 0.88845 92328 72256 99889 0.77459 66692 41483 37704 0.62110 29467 37226 40294 0.43424 37493 46802 55800 0.22338 66864 28966 88163 0.0	0.17001 71962 99402 603390(−01) 0.51603 28299 70797 396969(−01) 0.92927 19531 51245 376859(−01) 0.13441 52552 43784 220360 0.17151 19091 36391 380787 0.20062 85293 76989 021034 0.21915 68584 01587 496404 0.22551 04997 98206 687386
31	0.99909 81249 67667 59766 0.99383 19632 12755 02221 0.98153 11495 53740 10687 0.96049 12687 08020 28342 0.92965 48574 29740 05667 0.88845 92328 72256 99889 0.83672 59381 68868 73550 0.77459 66692 41483 37704 0.70249 62064 91527 07861 0.62110 29467 37226 40294 0.53131 97436 44375 62397 0.43424 37493 46802 55800 0.33113 53932 57976 83309 0.22338 66864 28966 88163 0.11248 89431 33186 62575 0.0	0.25447 80791 56187 441540(−02) 0.84345 65739 32110 624631(−02) 0.16446 04985 43878 109338(−01) 0.25807 59809 61766 535646(−01) 0.35957 10330 71293 220968(−01) 0.46462 89326 17579 865414(−01) 0.56979 50949 41233 574122(−01) 0.67207 75429 59907 035404(−01) 0.76879 62049 90035 310427(−01) 0.85755 92004 99903 511542(−01) 0.93627 10998 12644 736167(−01) 0.10031 42786 11795 578771 0.10566 98935 80234 809744 0.10957 84210 55924 638237 0.11195 68730 20953 456880 0.11275 52567 20768 691607

Continued

Table A.14. Patterson's Quadrature Rule, Continued.

n	Nodes $\pm x_k$	Weights w_k
63	0.99987 28881 20357 61194	0.36322 14818 45530 659694(-03)
	0.99909 81249 67667 59766	0.12651 56556 23006 801137(-02)
	0.99720 62593 72221 95908	0.25790 49794 68568 827243(-02)
	0.99383 19632 12755 02221	0.42176 30441 55885 483908(-02)
	0.98868 47575 47429 47994	0.61155 06822 11724 633968(-02)
	0.98153 11495 53740 10687	0.82230 07957 23592 966926(-02)
	0.97218 28747 48581 79658	0.10498 24690 96213 218983(-01)
	0.96049 12687 08020 28342	0.12903 80010 03512 656260(-01)
	0.94634 28583 73402 90515	0.15406 75046 65594 978021(-01)
	0.92965 48574 29740 05667	0.17978 55156 81282 703329(-01)
	0.91037 11569 57004 29250	0.20594 23391 59127 111492(-01)
	0.88845 92328 72256 99889	0.23231 44663 99102 694433(-01)
	0.86390 79381 93690 47715	0.25869 67932 72147 469108(-01)
	0.83672 59381 68868 73550	0.28489 75474 58335 486125(-01)
	0.80694 05319 50217 61186	0.31073 55111 16879 648799(-01)
	0.77459 66692 41483 37704	0.33603 87714 82077 305417(-01)
	0.73975 60443 52694 75868	0.36064 43278 07825 726401(-01)
	0.70249 62064 91527 07861	0.38439 81024 94555 320386(-01)
	0.66290 96600 24780 59546	0.40715 51011 69443 189339(-01)
	0.62110 29467 37226 40294	0.42877 96002 50077 344929(-01)
	0.57719 57100 52045 81484	0.44914 53165 36321 974143(-01)
	0.53131 97436 44375 62397	0.46813 55499 06280 124026(-01)
	0.48361 80269 45841 02756	0.48564 33040 66731 987159(-01)
	0.43424 37493 46802 55800	0.50157 13930 58995 374137(-01)
	0.38335 93241 98730 34692	0.51583 25395 20484 587768(-01)
	0.33113 53932 57976 83309	0.52834 94679 01165 198621(-01)
	0.27774 98220 21824 31507	0.53905 49933 52660 639269(-01)
	0.22338 66864 28966 88163	0.54789 21052 79628 650322(-01)
	0.16823 52515 52207 46498	0.55481 40435 65593 639878(-01)
	0.11248 89431 33186 62575	0.55978 43651 04763 194076(-01)
	0.05634 43130 46592 789972	0.56277 69983 12543 012726(-01)
	0.0	0.56377 62836 03847 173877(-01)

Continued

Table A.14. Patterson’s Quadrature Rule, Continued.

n	Nodes $\pm x_k$	Weights w_k
127	0.99998 24303 54891 59858	0.50536 09520 78625 176247(−04)
	0.99987 28881 20357 61194	0.18073 95644 45388 357820(−03)
	0.99959 87996 71910 68325	0.37774 66463 26984 660274(−03)
	0.99909 81249 67667 59766	0.63260 73193 62633 544219(−03)
	0.99831 66353 18407 39253	0.93836 98485 42381 500794(−03)
	0.99720 62593 72221 95908	0.12895 24082 61041 739210(−02)
	0.99572 41046 98407 18851	0.16811 42865 42146 990631(−02)
	0.99383 19632 12755 02221	0.21088 15245 72663 287933(−02)
	0.99149 57211 78106 13240	0.25687 64943 79402 037313(−02)
	0.98868 47575 47429 47994	0.30577 53410 17553 113613(−02)
	0.98537 14995 98520 37111	0.35728 92783 51729 964938(−02)
	0.98153 11495 53740 10687	0.41115 03978 65469 304717(−02)
	0.97714 15146 39705 71416	0.46710 50372 11432 174741(−02)
	0.97218 28747 48581 79658	0.52491 23454 80885 912513(−02)
	0.96663 78515 58416 56709	0.58434 49875 83563 950756(−02)
	0.96049 12687 08020 28342	0.64519 00050 17573 692280(−02)
	0.95373 00064 25761 13641	0.70724 89995 43355 546805(−02)
	0.94634 28583 73402 90515	0.77033 75233 27974 184817(−02)
	0.93832 03977 79592 88365	0.83428 38753 968157 70558(−02)
	0.92965 48574 29740 05667	0.89892 75784 06413 572328(−02)
	0.92034 00254 70012 42073	0.96411 77729 70253 669530(−02)
	0.91037 11569 57004 29250	0.10297 11695 79563 555237(−01)
	0.89974 4899 77694 003664	0.10955 73338 78379 016480(−01)
	0.88845 92328 72256 99889	0.11615 72331 99551 347270(−01)
	0.87651 34144 84705 26974	0.12275 83056 00827 700870(−01)
	0.86390 79381 93690 47715	0.12934 83966 36073 734547(−01)
	0.85064 44947 68350 27976	0.13591 57100 97655 467896(−01)
	0.83672 59381 68868 73550	0.14244 87737 29167 743063(−01)
	0.82215 62543 64980 40737	0.14893 64166 48151 820348(−01)
	0.80694 05319 50217 61186	0.15536 77555 58439 824399(−01)
	0.79108 49337 99848 36143	0.16173 21872 95777 199419(−01)
	0.77459 66692 41483 37704	0.16801 93857 41038 652709(−01)
	0.75748 39663 80513 63793	0.17421 93015 94641 737472(−01)
	0.73975 60443 52694 75868	0.18032 21639 03912 863201(−01)
	0.72142 30853 70098 91548	0.18631 84825 61387 901863(−01)

Continued

Table A.14. Patterson's Quadrature Rule, Continued.

n	Nodes $\pm x_k$	Weights w_k
	0.70249 62064 91527 07861	0.19219 90512 47277 660193(-01)
	0.68298 74310 91079 22809	0.19795 49504 80974 994880(-01)
	0.66290 96600 24780 59546	0.20357 75505 84721 594669(-01)
	0.64227 66425 09759 51377	0.20905 85144 58120 238522(-01)
	0.62110 29467 37226 40294	0.21438 98001 25038 672465(-01)
	0.59940 39302 42242 89297	0.21956 36630 53178 249393(-01)
	0.57719 57100 52045 81484	0.22457 26582 68160 987071(-01)
	0.55449 51326 31932 54887	0.22940 96422 93877 487608(-01)
	0.53131 97436 44375 62397	0.23406 77749 53140 062013(-01)
	0.50768 77575 33716 60215	0.23854 05210 60385 400804(-01)
	0.48361 80269 45841 02756	0.24282 16520 33365 993580(-01)
	0.45913 00119 89832 33287	0.24690 52474 44876 769091(-01)
	0.43424 37493 46802 55800	0.25078 56965 29497 687068(-01)
	0.40897 98212 29888 67241	0.25445 76996 54647 658126(-01)
	0.38335 93241 98730 34692	0.25791 62697 60242 293884(-01)
	0.35740 38378 31532 15238	0.26115 67337 67060 976805(-01)
	0.33113 53932 57976 83309	0.26417 47339 50582 599310(-01)
	0.30457 64415 56714 04334	0.26696 62292 74503 599062(-01)
	0.27774 98220 21824 31507	0.26952 74966 76330 319634(-01)
	0.25067 87303 03483 17661	0.27185 51322 96247 918192(-01)
	0.22338 66864 28966 88163	0.27394 60526 39814 325161(-01)
	0.19589 75027 11100 15392	0.27579 74956 64818 730349(-01)
	0.16823 52515 52207 46498	0.27740 70217 82796 819939(-01)
	0.14042 42331 52560 17459	0.27877 25147 66137 016085(-01)
	0.11248 89431 33186 62575	0.27989 21825 52381 597038(-01)
	0.84454 04008 37108 83710(-01)	0.28076 45579 38172 466068(-01)
	0.56344 31304 65927 89972(-01)	0.28138 84991 56271 506363(-01)
	0.28184 64894 97456 94339(-01)	0.28176 31903 30166 021307(-01)
	0.0	0.28188 81418 01923 586938(-01)

Table A.15. Filon’s Quadrature Formula.

θ	α	β	γ
0.00	0.0	0.66666 667	1.33333 333
0.01	0.00000 004	0.66668 000	1.33332 000
0.02	0.00000 036	0.66671 999	1.33328 000
0.03	0.00000 120	0.66678 664	1.33321 334
0.04	0.00000 284	0.66687 990	1.33312 001
0.05	0.00000 555	0.66699 976	1.33300 003
0.06	0.00000 961	0.66714 617	1.33285 340
0.07	0.00001 524	0.66731 909	1.33268 012
0.08	0.00002 274	0.66751 844	1.33248 020
0.09	0.00003 237	0.66774 417	1.33225 365
0.1	0.00004 438	0.66799 619	1.33200 048
0.2	0.00035 354	0.67193 927	1.32800 761
0.3	0.00118 467	0.67836 065	1.32137 184
0.4	0.00278 012	0.68703 909	1.31212 154
0.5	0.00536 042	0.69767 347	1.30029 624
0.6	0.00911 797	0.70989 111	1.28594 638
0.7	0.01421 151	0.72325 813	1.26913 302
0.8	0.02076 156	0.73729 136	1.24992 752
0.9	0.02884 683	0.75147 168	1.22841 118
1.0	0.03850 188	0.70525 831	1.20467 472

Table A.16. Gauss-Cos Quadrature on $[-\pi/2, \pi/2]$.

n	Nodes $\pm x_k$	Weights w_k
2	0.68366 73900 89903 04094	1.0
4	0.43928 74668 60015 14756 0.11906 76563 89485 57415(+01)	0.77592 93818 72379 83935 0.22407 06181 27620 16065
8	0.25649 65074 16231 23020 0.743468 64787 54924 4989 0.11537 25645 45672 75850(+01) 0.14414 90540 18235 75701(+01)	0.49199 57966 03200 88314 0.33626 44778 52804 59621 0.14420 40920 30227 50950 0.27535 63351 37670 11149(−01)
16	0.14003 44442 46967 73778 0.41577 19167 34189 43962 0.61861 10809 75605 45347 0.92027 18620 66370 96491 0.11330 06878 60050 03695(+01) 0.13091 81890 44529 36698(+01) 0.14446 01487 36665 14608(+01) 0.15321 50113 23623 04719(+01)	0.27661 09576 48260 50408 0.24763 63209 46355 22403 0.19741 14887 02534 55567 0.13834 19552 69512 73359 0.83026 64757 32177 42131(−01) 0.40437 89394 65036 69410(−01) 0.14115 26815 68540 08264(−01) 0.24194 67756 76156 28193(−02)

Table A.17. Gauss-Cos Quadrature on $[0, \pi/2]$.

n	Nodes $\pm x_k$	Weights w_k
2	0.26587 38805 63078 23382 0.10351 52609 31713 15182(+01)	0.60362 55328 08271 13087 0.39637 44671 91728 86913
4	0.95669 38919 68586 36773(-01) 0.45240 90232 70670 96554 0.93185 05767 20240 82424 0.13564 43959 96664 66230(+01)	0.23783 07141 95155 04517 0.40265 69552 35812 53512 0.28681 73794 85647 15225 0.72694 95108 33852 67446(-01)
8	0.29023 72976 89139 33432(-01) 0.14828 52440 458181 9442 0.34531 11115 16647 87488 0.59447 69679 76583 60178 0.86538 38068 61235 04827 0.11263 07609 31874 56632(+01) 0.13470 15046 02812 58016(+01) 0.15015 60362 20591 95568(+01)	0.73908 99809 51173 84985(-01) 0.16002 99370 23380 06099 0.21444 43434 18035 49108 0.21979 58126 88519 03339 0.17581 16447 82095 68886 0.10560 44802 53083 22171 0.42485 49729 92172 01089(-01) 0.79192 86440 55191 78899(-02)
16	0.80145 03490 62959 73494(-02) 0.41893 03135 42462 54797(-01) 0.10149 95448 67575 79459 0.18463 18592 38366 17507 0.28826 38848 77605 74589 0.40870 79076 46479 41910 0.54176 05498 69138 47463 0.68287 63665 87194 16893 0.82729 28762 04168 33520 0.97018 21259 48293 67065 0.11067 86515 02862 47873(+01) 0.12325 55569 72277 48824(+01) 0.13432 82192 15807 21861(+01) 0.14352 37054 92950 32923(+01) 0.15052 97087 67946 69248(+01) 0.15510 58694 40861 35769(+01)	0.20528 71497 72152 48902(-01) 0.46990 91985 35979 58123(-01) 0.71441 02131 22185 41698(-01) 0.92350 33832 92430 52271(-01) 0.10804 92802 68162 36935 0.11698 24124 33062 61791 0.11812 39536 17620 37649 0.11137 58494 04200 91049 0.97778 23614 59465 43110(-01) 0.79418 75898 59444 82077(-01) 0.59039 62005 37686 91402(-01) 0.39458 87678 37281 65671(-01) 0.22987 78567 72068 47531(-01) 0.11010 40560 04215 36861(-01) 0.38123 92803 04999 15653(-02) 0.65143 37546 12666 56171(-03)

Table A.18. Coefficients in (5.1.15) with $w(x) = \ln(1/x)$, $0 < x < 1$.

n	α_n	β_n
0	0.25	0.0
1	0.464285714286	0.486111111111(−1)
2	0.485482446456	0.586848072562(−1)
3	0.492103081871	0.607285839189(−1)
4	0.495028498758	0.614820201969(−1)
5	0.496579511644	0.614808095319(−1)
6	0.497501301305	0.620390629544(−1)
7	0.498094018204	0.621599191583(−1)
8	0.498494018204	0.622389376716(−1)
9	0.498785322656	0.622933886799(−1)
10	0.498997353167	0.623324775066(−1)
11	0.499158221678	0.623614734838(−1)
12	0.499283180126	0.623835683595(−1)
13	0.499382187671	0.624007864342(−1)
14	0.499461972097	0.624144615353(−1)
15	0.499527212427	0.624255013029(−1)
16	0.499581244730	0.624345406235(−1)
17	0.499626499806	0.624420343142(−1)
18	0.499664782928	0.624483150597(−1)
19	0.499697457641	0.624536307243(−1)

Table A.19. Coefficients in (5.1.15) with $w(x) = E_1(x)$, $0 < x < \infty$.

n	α_n	β_n
0	0.5	0.0
1	0.23(+1)	0.416666666667
2	0.423469387755(+1)	0.261333333333(+1)
3	0.619917288995(+1)	0.675494793836(+1)
4	0.817602876377(+1)	0.128700101592(+2)
5	0.101592444559(+2)	0.209689946964(+2)
6	0.121467630339(+2)	0.310570066309(+2)
7	0.141367011214(+2)	0.431369541345(+2)
8	0.161284556528(+2)	0.572106684370(+2)
9	0.181215390823(+2)	0.732793862452(+2)
10	0.201156292899(+2)	0.913439870981(+2)
11	0.221105037868(+2)	0.111405121907(+3)
12	0.241060033128(+2)	0.133463287826(+3)
13	0.261020104696(+2)	0.157518874426(+3)
14	0.280984365631(+2)	0.183572193521(+3)
15	0.300952131707(+2)	0.211623499185(+3)
16	0.320922865502(+2)	0.241673001620(+3)
17	0.340896138248(+2)	0.273710877032(+3)
18	0.360861603136(+2)	0.307767274831(+3)
19	0.380848976220(+2)	0.343812322983(+3)

Table A.20. 10-point Gauss-Christoffel Rule
with $w(x) = \ln(1/x)$, $0 < x < 1$.

ξ_i	λ_i
0.904263096219(-2)	0.120955131955
0.539712662225(-1)	0.186363542564
0.135311824639	0.195660873278
0.247052416287	0.173577142183
0.380212539609	0.135695672995
0.523792317972	0.936467585381(-1)
0.665775205517	0.557877273514(-1)
0.794190416012	0.271598108992(-1)
0.898161091219	0.951518260284(-2)
0.968847988719	0.163815763360(-2)

Table A.21. 20-point Gauss-Christoffel Rule
with $w(x) = \ln(1/x)$, $0 < x < 1$.

ξ_i	λ_i
0.255832795592(−2)	0.431427521332(−1)
0.152096623496(−1)	0.753837099086(−1)
0.385365503721(−1)	0.930532674517(−1)
0.721816138158(−1)	0.101456711850
0.115460526488	0.103201762056
0.167442856275	0.100022549805
0.226983787260	0.932597993003(−1)
0.292754960941	0.840289528792(−1)
0.363277429858	0.732855891300(−1)
0.436957140091	0.618503369137(−1)
0.512122594679	0.504166044385(−1)
0.587064044915	0.395513700052(−1)
0.661173413315	0.296940778958(−1)
0.729484083930	0.211563153554(−1)
0.793709671987	0.141237329390(−1)
0.851280892789	0.866097450433(−2)
0.900879680854	0.471994014620(−2)
0.941369749129	0.215139740396(−2)
0.971822741075	0.719728214653(−3)
0.991538081439	0.120427676330(−3)

Table A.22. 10-point Gauss-Christoffel Rule
with $w(x) = E_1(x)$, $0 < x < \infty$.

ξ_i	λ_i
0.762404872624(−1)	0.485707599602
0.525005762690	0.357347318586
0.143921959617(+1)	0.127767083774
0.286324173848(+1)	0.263265788641(−1)
0.484664684765(+1)	0.314097760897(−2)
0.745940513320(+1)	0.203866802942(−3)
0.108101228402(+2)	0.648957008433(−5)
0.150823083551(+2)	0.848669062576(−7)
0.206311914914(+2)	0.324960593979(−9)
0.283693946254(+2)	0.156050745676(−12)

Table A.23. 20-point Gauss-Christoffel Rule
with $w(x) = E_1(x)$, $0 < x < \infty$.

ξ_i	λ_i
0.415731018684(-1)	0.330068388136
0.274239640181	0.335018800621
0.735213024633	0.202727089842
0.143646482057(+1)	0.906794137819(-1)
0.238684236390(+1)	0.311926475044(-1)
0.359494938617(+1)	0.830681682460(-2)
0.507042045480(+1)	0.170519552143(-2)
0.682474522008(+1)	0.267192385286(-3)
0.887199456612(+1)	0.315225257509(-4)
0.112296313102(+2)	0.275116436420(-5)
0.139195560950(+2)	0.173736449646(-6)
0.169695733188(+2)	0.771970107104(-8)
0.204155650908(+2)	0.232856519853(-9)
0.243048836079(+2)	0.454955059531(-11)
0.287019535563(+2)	0.540355193304(-13)
0.336981998188(+2)	0.356730027303(-15)
0.394313665944(+2)	0.114479498566(-17)
0.461284475183(+2)	0.143415823640(-20)
0.542229680449(+2)	0.463374056293(-24)
0.648259442473(+2)	0.136239857196(-28)

Table A.24. Sidi's Nodes $x_{k,i}$ for $w(x) = (1 - x)^\alpha x^\beta (\log x)^\nu$.

k	$x_{k,i}$
2	0.1504720765483788247340868(+0)
	0.7384168123405100425671321(+0)
3	0.4966471483058575164815096(-1)
	0.3733950309821642554730659(+0)
	0.8425652541872500345121466(+0)
4	0.1799068499801418849481927(-1)
	0.1834165223808434663776978(+0)
	0.5414157204189523620030400(+0)
	0.8955770722021899610254536(+0)
5	0.6965462488720096032035478(-2)
	0.9279357371061748571694494(-1)
	0.3274158560864037226245671(+0)
	0.6563187419838211189571098(+0)
	0.9258942258127421665037105(+0)
6	0.2826962449669843599475705(-2)
	0.4862455152896217464020268(-1)
	0.1976882676470386179801153(+0)
	0.4503451521122742717828658(+0)
	0.7351670962539651466016721(+0)
	0.9447647096318861903441189(+0)
7	0.1187258545164058707796495(-2)
	0.2628663472239343296132930(-1)
	0.1210706424838506878316480(+0)
	0.3040908096207194377669225(+0)
	0.5483105637900639317550144(+0)
	0.7906485354805576903913789(+0)
	0.9572768818037840077295186(+0)
8	0.5115121670143565456995161(-3)
	0.1458573317963311050116104(-1)
	0.7546523540379770911279422(-1)
	0.2056995360684232831971485(+0)
	0.3998834536687977392332982(+0)
	0.6250150234434243001757636(+0)
	0.8308072107358005498056741(+0)
	0.9659870403646759751126183(+0)

Continued

Table A.24. Sidi's Nodes $x_{k,i}$ for $w(x) = (1-x)^\alpha x^\beta (\log x)^\nu$, Continued.

k	$x_{k,i}$
9	0.2247255954393555916169534(-3)
	0.8269188094627755516996537(-2)
	0.4785186222081606877143400(-1)
	0.1402987492166232474932741(+0)
	0.2900554492782025373109889(+0)
	0.4820003130318437634116435(+0)
	0.6851379193950803969670460(+0)
	0.8606574901008240408017969(+0)
	0.9722887040665427749175365(+0)
10	0.1002519058889115183838894(-3)
	0.4772351178865461701628092(-2)
	0.3081710497452419192376816(-1)
	0.09668389372266823766910449(+0)
	0.2108292927888059664631726(+0)
	0.3681879873486372245494636(+0)
	0.5510145152797366607799745(+0)
	0.7326572440917100692558961(+0)
	0.8833778455567603549170030(+0)
11	0.9769924074477204234412397(+0)
	0.4527279518770788580960679(-4)
	0.2795480278297609710164151(-2)
	0.2012015530035912019846123(-1)
	0.6733379444645636036081982(-1)
	0.1540683692211295141571981(+0)
	0.2806977184599954155963530(+0)
	0.4379750731607002234291315(+0)
	0.6086538380237029866037801(+0)
12	0.7706276021403856146818612(+0)
	0.9010352101154075477040806(+0)
	0.9805950222280231942661999(+0)
	0.2064864876175711460486520(-4)
	0.1658119145275128080915805(-2)
	0.1329440070499037472584458(-1)
	0.4736615645452630501965885(-1)
	0.1133435389770539175602337(+0)
	0.2143947425636104353596778(+0)
	0.3465368850551303059326358(+0)
	0.4991909417699800788348341(+0)
	0.6568098047861666843871831(+0)
	0.8013203430670089444376458(+0)
	0.9150102643845973160452445(+0)
	0.9834146345679861678235056(+0)

Table A.25. Nodes $x_{k,i}$ for Sidi’s Rule \bar{S}_k .

k	$x_{k,i}$
2	0.3333333333333333148296163(+0)
	0.1(+1)
3	0.1078176738977890680715177(+0)
	0.5796823261022109319284823(+0)
	0.2915970806672432691364349(+0)
	0.7182032643371645264096514(+0)
	0.1(+1)
5	0.1454539367063958053838402(−1)
	0.1476352319507779342622200(+0)
	0.4492290509129626685513870(+0)
	0.7998557555643852623461498(+0)
	0.1(+1)
6	0.5833465496275194034359046(−2)
	0.7697070383625363720891954(−1)
	0.2741621191525560052859589(+0)
	0.5678514494337698614856436(+0)
	0.8511684583089076383544125(+0)
	0.1(+1)
7	0.2429255658444682414165428(−2)
	0.4135196615566082145587501(−1)
	0.1682791497337559616376268(+0)
	0.3890765863668857460488937(+0)
	0.6551717852719092238800158(+0)
	0.8852584870379529569106580(+0)
	0.1(+1)
8	0.1040274764820644419829887(−2)
	0.2280766587902437192436622(−1)
	0.1047703618903654126937042(+0)
	0.2647931716598577733812192(+0)
	0.4853839359718086776673829(+0)
	0.7199405641129489330509728(+0)
	0.9089631138816870459251618(+0)
	0.1(+1)

Continued

Table A.25. Nodes $x_{k,i}$ for Sidi's Rule \bar{S}_k , Continued.

n	$x_{n,i}$
9	0.4550296440994962016840519(−3)
	0.1286108481364281637404634(−1)
	0.6627059781567289087345074(−1)
	0.1809718441335950167569990(+0)
	0.3548946891567039685355667(+0)
	0.5639126195922897766266146(+0)
	0.7687669484229625593840751(+0)
	0.9260720764210335076427327(+0)
	0.1(+1)
10	0.2023447402752151231923594(−3)
	0.7387651749525755116854153(−2)
	0.4255601458052361146799925(−1)
	0.1247171375024214851068294(+0)
	0.2589708071707655934190484(+0)
	0.4345652946896826906986178(+0)
	0.6275259400042944024633584(+0)
	0.8062449296905893625364570(+0)
	0.9388060635967709899318834(+0)
	0.1(+1)

Table A.26. Nodes $x_{k,i}$ for Sidi’s Rule S_k .

k	$x_{k,i}$
2	0.1352966685416368830541245(+0)
	1.642481109236140879303889(+0)
3	0.4505096041273612406108384(−1)
	0.6767167970341259053412841(+0)
	0.3075107242553138053864359(+1)
4	0.1666747355483805953513254(−1)
	0.3180181842758116328440110(+0)
	0.1552471013121895948572160(+1)
	0.4666443329047454291469421(+1)
5	0.6575286461353594714973614(−2)
	0.1606142317401454133740657(+0)
	0.8655532227468952788385081(+0)
	0.2654640475454163262014617(+1)
	0.6359556084008965548548531(+1)
6	0.2707864701816735299860772(−2)
	0.8508305148428640940494461(−1)
	0.5092057433688204071131622(+0)
	0.1639972558714133166191118(+1)
	0.3915248557178793831212715(+1)
	0.8124282662294927348511919(+1)
7	0.1149791448528518413713106(−2)
	0.4664783979294682969563013(−1)
	0.3106265453447279445420293(+0)
	0.1058211225813305400578201(+1)
	0.2590541885281939293861342(+1)
	0.5292380339780669906701860(+1)
	0.9942541657663614529383267(+1)
8	0.4994312298446428261336494(−3)
	0.2624962191042572168253599(−1)
	0.1946430851588193677859095(+0)
	0.7030609671769538771002317(+0)
	0.1779188598644186436459336(+1)
	0.3678545091181902204624521(+1)
	0.6758890871288327772958837(+1)
	0.1180256029366207570774350(+2)

Continued

Table A.26. Nodes $x_{k,i}$ for Sidi's Rule S_k , Continued.

k	$x_{k,i}$
9	0.2207521317724925791117080(−3)
	0.1507552393251116763794872(−1)
	0.1245393110961793281532550(+0)
	0.4773846078371063450518363(+0)
	0.1252523841360254186483303(+1)
	0.2642940899971808033086518(+1)
	0.4875885820583371277336937(+1)
	0.8296284357470376846777071(+1)
	0.1369620449461662126111605(+2)
10	0.9892395934261595503121656(−4)
	0.8801264957863189422604400(−2)
	0.8103177761469819440076634(−1)
	0.3297575418975984273828317(+0)
	0.8980931136795896607694090(+0)
	0.1940497820366211545461965(+1)
	0.3624993110444317157003979(+1)
	0.6162058054822851183018884(+1)
	0.9891400587100292796094436(+1)
11	0.1561759674811040987663091(+2)
	0.4482320342657574276708926(−4)
	0.5207909623162271066376672(−2)
	0.5345475360211059123738409(−1)
	0.2309906558108135166129671(+0)
	0.6533678661614568117244062(+0)
	0.1447701829626337088896548(+1)
	0.2748104892732672333011124(+1)
	0.4705876379525167685358156(+1)
12	0.7521799853246243117155245(+1)
	0.1153453533217644455532991(+2)
	0.1756233860215826325656963(+2)
	0.2049481473588502707387955(−4)
	0.3116434971088132607069943(−2)
	0.3567129378808611001039353(−1)
	0.1637038106438552242938300(+0)
	0.4810226336846232242372423(+0)
	0.1093749789758291512953292(+1)
	0.2113272551481096162007134(+1)
	0.3658647547020350998536742(+1)
	0.5870258102208375738939594(+1)
	0.8943499910675443587138034(+1)
	0.1321831883068720792095974(+2)
	0.1952704436176789215551253(+2)

Table A.27. Sidi's Quadrature Rules.

The nodes $x_{k,i}$ of Sidi's formulas $\int_0^\infty w(x) f(x) dx \approx \sum_{i=1}^k A_{k,i} f(x_i)$, where $w(x) = x^\alpha e^{-x}$ (Case 1), or $w(x) = x^\alpha E_p(x)$, $p > 1$ (Case 2), are given below. The weights $A_{k,i}$ for these two cases are given separately, but the nodes remain the same in both cases.

k	Nodes $x_{k,i}$	Weights $A_{k,i}$ (Case 1)
2	0.13529666851116368734312115 0.16424811092361409043110506(+01)	0.7580234232710699835513690 0.2419765767289300164486310
3	0.4505096041273612628731663(−01) 0.6767167970341259016621497 0.3075107242553137972050534(+01)	0.4554540735108335506704450 0.4982740688105893984787207 0.4627185767857705085083424(−01)
4	0.1666747355483805876646528(−01) 0.3180181842758116537606890 0.1552471013121895871047765(+01) 0.4666443329047454410425080(+01)	0.2559124314488475647034520 0.5540725756664822258223339 0.1821354548398085887398495 0.7879538044861620734364579(−02)
5	0.6575286461353594336586520(−02) 0.1606142317401454028672786 0.8655532227468952548875133 0.2654640475454163235703710(+01) 0.6359556084008965145949766(+01)	0.1402073401311772741711620 0.4891155383497700586633836 0.3175517522863648430356046 0.5187500819320468386324305(−01) 0.1250361039483140266606736(−02)
6	0.2707864701816735328121392(−02) 0.8508305148428640858724367(−01) 0.5092057433688204133906909 0.1639972558714133179393992(+01) 0.3915248557178793725173108(+01) 0.8124282662294926782302315(+01)	0.7590679384919516304074620(−01) 0.3882569073353100374747409 0.3910982789957450034559817 0.1317949666122117178283279 0.1275405893635085165625092(−01) 0.1889942711872265439523386(−03)
7	0.1149791448528518322907199(−02) 0.4664783979294682653256681(−01) 0.3106265453447279364212658 0.1058211225813305334731752(+01) 0.2590541885281939341616039(+01) 0.5292380339780669851059954(+01) 0.9942541657663614613190516(+01)	0.4081165699922444055525246(−01) 0.2916484563421986709994837 0.4031742897215124443059980 0.2164039357580742197306810 0.4509850270751601688195192(−01) 0.2535608913318645418197694(−02) 0.2754955815556210853516167(−04)

Continued

Table A.27. Sidi's Quadrature Rules, Continued.

k	Nodes $x_{k,i}$	Weights $A_{k,i}$ (Case 1)
8	0.4994312298446427845065726(−03)	0.2183694095237601731347362(−01)
	0.2624962191042572294099059(−01)	0.2123436066706023280859898
	0.1946430851588193647017747	0.3759015998592184903536997
	0.7030609671769538287123412	0.2797841689691778014757056
	0.1179188598644186365876674(+01)	0.9604431756368414199484653(−01)
	0.3678545091181902027940886(+01)	0.1350041606147886266984887(−01)
	0.6758890871288327828074605(+01)	0.5850466653776554364622037(−03)
	0.1180256029366207606252295(+02)	0.3903258084702669973656278(−05)
9	0.2207521317724925858938488(−03)	0.1163948148700660433391451(−01)
	0.1507552393251116722526709(−01)	0.1517165526134532491022856
	0.1245393110961793261601531	0.3298341874710617676412120
	0.4773846078371063555094626	0.3135048910910120987495115
	0.1252523841360254225620565(+01)	0.1530007866011305814318330
	0.2642940899971808063081664(+01)	0.3653427788604604752980879(−01)
	0.4675885820583371555261397(+01)	0.3655427407496274166283388(−02)
	0.8296284357470376096847307(+01)	0.1138550570413118897646681(−03)
10	0.1369620449461662071770829(+02)	0.5403857520651553866290788(−06)
	0.9892395934161595489626947(−04)	0.6183607395711354252866023(−02)
	0.8801264957863189992681821(−02)	0.1071091101886063889549707
	0.8103177761469819944716406(−01)	0.2784453407952368949679836
	0.3297575418975984320679508	0.3208016909050212375820361
	0.8980931136795896724077270	0.2033397579357152368218497
	0.1940497820366211633196074(+01)	0.7082269642288027252226315(−01)
	0.3624993110444317167348184(+01)	0.1236216945865997469233175(−01)
	0.6162058054822850870745952(+01)	0.9144211000825651826936216(−03)
	0.9891400587100193449508436(+01)	0.2113241163514073803417835(−04)
	0.1561759674811040950577130(+02)	0.7338645093400497129421534(−07)

Continued

Table A.27. Sidi’s Quadrature Rules, Continued.

k	Nodes $x_{k,i}$	Weights $A_{k,i}$ (Case 1)
11	0.4482320342657574489567133(−04)	0.3275384530104277670283281(−02)
	0.5207909623162271469395125(−02)	0.7501957741413657025016744(−01)
	0.5345475360211059413823949(−01)	0.2291117291836910307454911
	0.2309906558108135273776385	0.3090943534216158917513319
	0.6533678661614567980364082	0.2398422278869326897396240
	0.1447701829626337013453597(+01)	0.1107670005330865349182265
	0.2748104892732672279111629(+01)	0.2886106586282509163584454(−01)
	0.4705876379525167924577051(+01)	0.3810438741749370467894437(−02)
	0.7521799853246242986333288(+01)	0.2144416921941403642591808(−03)
	0.1153453533217644513798817(+02)	0.3770931329409887434130059(−05)
	0.1756233860215826167109416(+02)	0.9804334992569433381436212(−08)
12	0.2049481473588502838963231(−04)	0.1730217229647563323727468(−02)
	0.3116434971088132598181122(−02)	0.5225852598266425798596882(−01)
	0.3567129378808611226048581(−01)	0.1852238054344086666606745
	0.1637038106438552243872225	0.2857579736265443988113541
	0.4810226336846232187336123	0.2607043547367742704644881
	0.1093749789758291561354613(+01)	0.1497818572726624001050412
	0.2113272551481096111677349(+01)	0.5279170686778839885617192(−01)
	0.3658647547020350981572865(+01)	0.1061556042946016328951724(−01)
	0.5870258102208375884709533(+01)	0.1087699857196495210286065(−02)
	0.8943499910675444211687219(+01)	0.4764646687998658382098453(−04)
	0.1321831883068720803236893(+02)	0.6508045093724211033391325(−06)
	0.1952704436176789300899542(+02)	0.1291464026287846155793969(−08)

Continued

Table A.27. Sidi's Quadrature Rules with Weights $A_{k,i}$ (Case 2), Continued.

k	Weights $A_{k,i}$ (Case 2)
2	0.7580234232710699835513690 0.2419765767289300164486310
3	0.4554540735108335506704450 0.4982740688105893984787207 0.4627185767857705085083424(-01)
4	0.2559124314488475647034520 0.5540725756664822258223339 0.1821354548398085887398495 0.7879538044861620734364579(-02)
5	0.1402073401311772741711620 0.4891155383497700586633836 0.3175517522863648430356046 0.5187500819320468386324305(-01) 0.1250361039483140266606738(-02)
6	0.7590679384919516304074620(-01) 0.3882569073353100374747409 0.3910982789957450034559817 0.1317949666122117178283279 0.1275405893635085165625092(-01)
7	0.4081165699922444055525246(-01) 0.2916484563421986709994837 0.4031742897215124443059980 0.2164039357580742197306810 0.4509850270751601688195192(-01) 0.2835608913318645418197694(-02) 0.2154955815556210843516167(-04)
8	0.2183694095237601731347362(-01) 0.2123436066706023280859898 0.3759015998592184903336997 0.2797841689691778014757056 0.9604431756368414199484653(-01) 0.1350041606147886266984887(-01) 0.5850466653776554364622037(-03) 0.3903258084702669973656278(-05)
9	0.1163948148700660433391451(-01) 0.1517165526134532491022856 0.3298341874710617676412120 0.3135048910910120987495115 0.153000786601130581Q318330 0.3653427788604604752980879(-01) 0.3655427407496274166283388(-02) 0.1138550570413118897646681(-03) 0.5403857520651553866290788(-06)

Continued

Table A.27. Sidi’s Quadrature Rules with Weights $A_{k,i}$ (Case 2), Continued.

k	Weights $A_{k,i}$ (Case 2)
10	0.6183607395711354532866023(−02)
	0.1071091101886063889549707
	0.2784453407952368949679836
	0.3208016909050212375820361
	0.2033397579357152368218497
	0.7082269642288027252226315(−01)
	0.1236216945865997469233175(−01)
	0.9144211000825651826936216(−03)
	0.2113241163514073803417835(−04)
	0.7338645093400497129421534(−07)
11	0.3275384530104277670293281(−02)
	0.7501957741413657025016744(−01)
	0.2291117291836910307454911
	0.3090943534216158917513319
	0.2398422278869326897396240
	0.1107670005330865349182265
	0.2886106586082509163584454(−01)
	0.3810438741749370467894437(−02)
	0.2144416921941403642591808(−03)
	0.3770931329409887434130059(−05)
	0.9804334992569433381436212(−08)
12	0.1730217229647563323727468(−02)
	0.5225852598266425798596882(−01)
	0.1852238054344086666606745
	0.2857579736265443988113541
	0.2607043547367742704644881
	0.1497818572726624001050412
	0.5279170686778839885617192(−01)
	0.1061556042946016328951724(−01)
	0.1087699857196495210286065(−02)
	0.4764646687998658382098453(−04)
	0.6508045093724211033391325(−05)
	0.1291464026287846155793969(−08)

Table A.28. Values of B_j defined in (7.2.5).

	D_0	D_1	D_2	D_3	D_4	D_5
B_0	1	0	0	0	0	0
B_1	-2.5	2.5	0	0	0	0
B_2	3.375	-11.5	7.875	0	0	0
B_3	-4.0625	28.4375	-51.1875	26.8125	0	0
B_4	4.6484375	-55.78125	184.078125	-227.90625	94.960903	0
B_5	-5.1679688	99.746094	-164.22656	1055.7422	-997.08984	344.44922

Table A.29. Values of C_n , $n = 0(1)10$, defined by (7.2.17).

n	C_0	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}
0	1										
1	1	1									
2	2	3	1								
3	5	9	5	1							
4	14	28	20	7	1						
5	42	90	75	35	9	1					
6	132	297	275	154	54	11	1				
7	429	1001	1001	637	273	77	13	1			
8	1430	3432	3640	2548	1260	440	104	15	1		
9	4862	11934	13260	9996	5508	2244	663	135	17	1	
10	16796	41990	48450	38760	23256	10659	3705	950	170	19	1

Table A.30. Coefficients of $\phi_k^{(N)}(x)$.

N	k	1	x	x^2	x^3	x^4	x^5	x^6
3	1	9	-36	30				
	2	-36	192	-180				
	3	30	-180	180				
4	1	16	-120	240	-140			
	2	-120	1200	-2700	1680			
	3	240	-2700	6480	-4200			
	4	-140	1680	-4200	2800			
5	1	25	-300	1050	-1400	630		
	2	-300	4800	-18900	26880	-12600		
	3	1050	-18900	79380	-117600	56700		
	4	-1400	26880	-117600	179200	-88200		
	5	630	-12600	56700	-88200	44100		
6	1	36	-630	3360	-7560	7560	-2772	
	2	-630	14700	-88200	211680	-220500	83160	
	3	3360	-88200	564480	-1411200	1512000	-582120	
	4	-7560	211680	-1411200	3628800	-3969000	1552320	
	5	7560	-220500	1512000	-3969000	4410000	-1746360	
	6	-2772	83160	-582120	1552320	-1746340	698544	
7	1	49	-1176	8820	-29400	48510	-38808	12012
	2	-1176	37632	-317520	1128960	-1940400	1596672	-504504
	3	8820	-317520	2857680	-10584000	18711000	-15717240	5045040
	4	-29400	1128960	-10584000	40320000	-72765000	62092800	-20180160
	5	48510	-1940400	18711000	-72765000	133402500	-115259760	37837800
	6	-38808	1596672	-15717240	62092800	-115259760	100590336	-33297264
	7	12012	-504504	5045040	-20180160	37837800	-33297264	11099088

Table A.31. Nodes and Weights for the G_N^* -Rule.

For $N = 2$, the nodes are:

0.18829 87963 117412(+1) + i 0.32447 96910 641054(+1)
 0.20000 00000 000000(+1) + i 0.14142 13562 373095(+1)
 0.30082 17622 152272(+1) + i 0

and the corresponding weights are:

−0.88899 04409 694117(+0) + i 0.40706 16686 678985(+0)
 0.39225 87291 528748(−1) + i 0.26865 36655 316489(+0)
 0.26995 29136 108248(+1) + i 0.

Table A.32. Values of p_j .

n, k	j	p_j
40, 40	1	462.1042859692760191(+19)
40, 39	2	−1.3818144531579131(+21)
40, 38	3	4.3564892136190142(+22)
40, 19	22	−2.0943817887520176(+33)
40, 18	23	2.5922682191202954(+33)
40, 17	24	−2.8444833911749354(+33)
40, 16	25	2.7628672917493189(+33)
40, 15	26	−2.3699585982237493(+33)
35, 4	227	−1.2593960730679819(+24)
35, 3	228	1.4372550728020953(+23)
35, 2	229	−1.1487452598211684(+22)
2, 1	857	4.3726366344881985(−14)
2, 0	858	−1.8030596495382691(−15)
1, 1	859	5.4318417593283853(−16)
1, 0	860	−3.3531316106852708(−17)
0, 0	861	−4.6289996351134026(−19)

B

Figures

Figures mentioned in the book are collected here for reference. They are not essential for the exposition of the text, although they may provide some visual aid to the subject matter.

Chapter 2

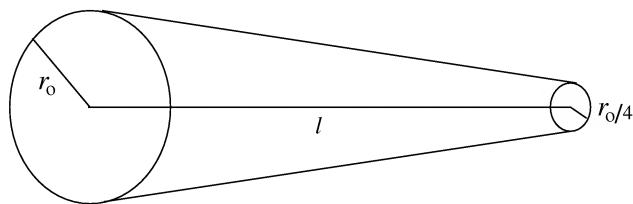


Fig. 2.7.1.

Chapter 7

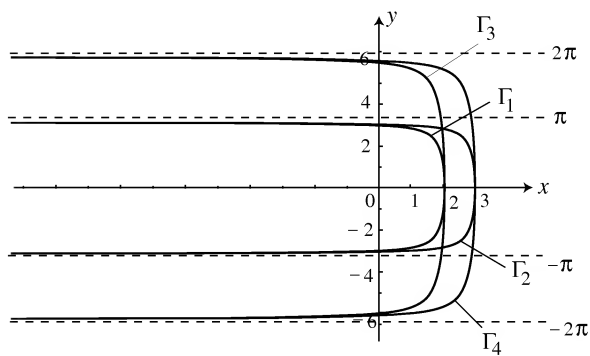


Fig. 7.5.1. Tablot Contours

Chapter 8

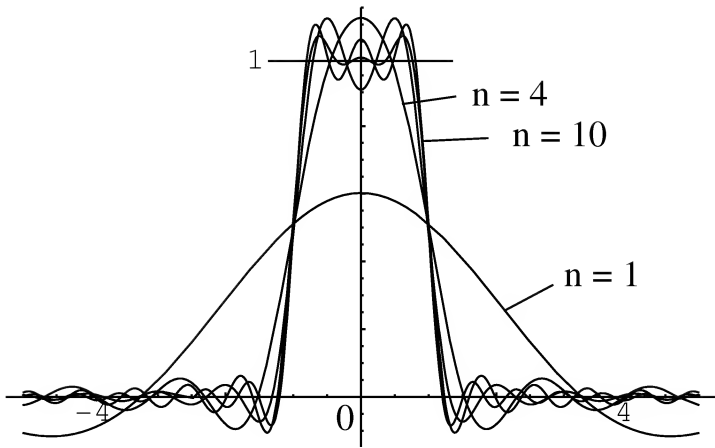
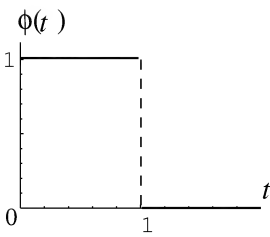
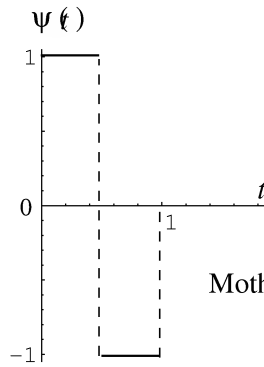


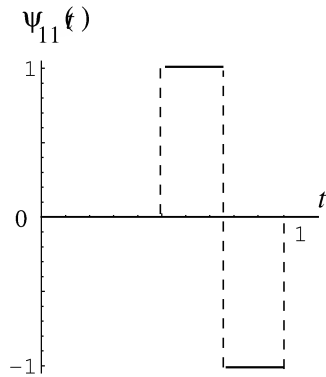
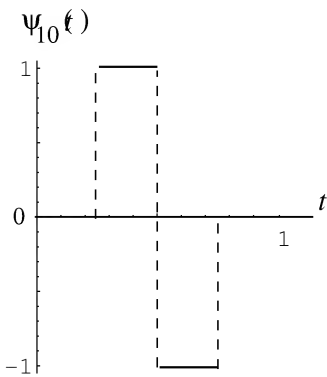
Fig. 8.2.1. Gibbs Phenomenon.



Father Wavelet

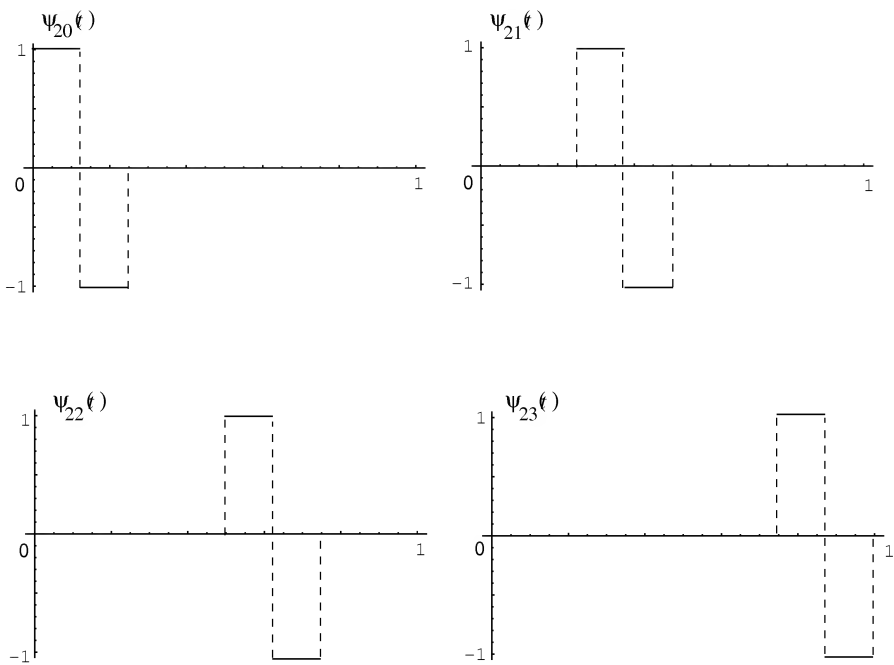


Mother Wavelet

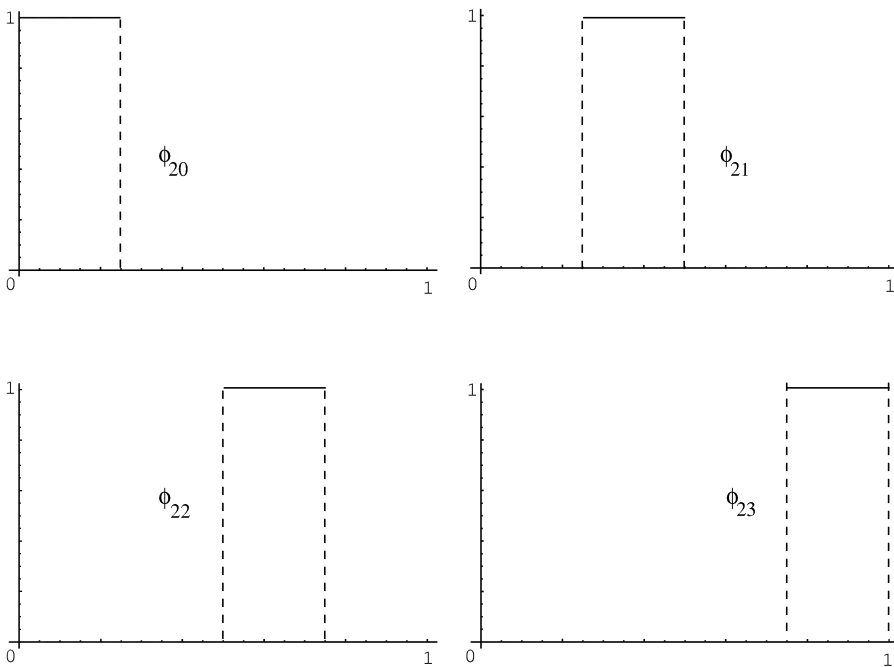


First Generation Haar Daughter Wavelets

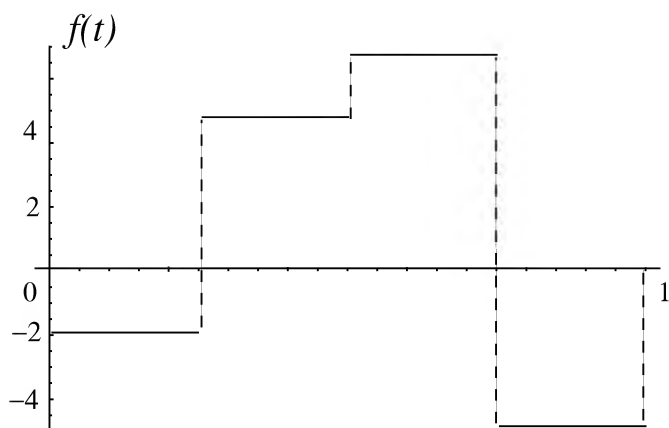
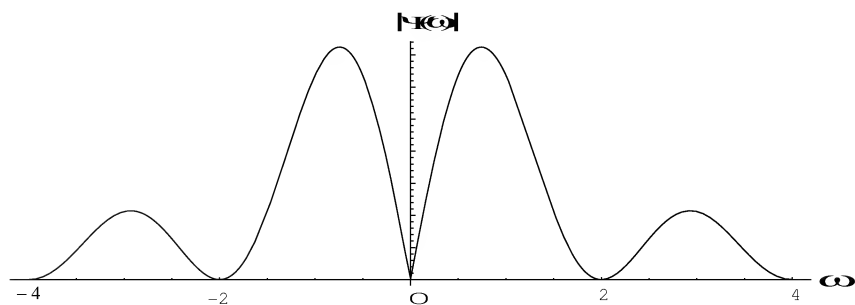
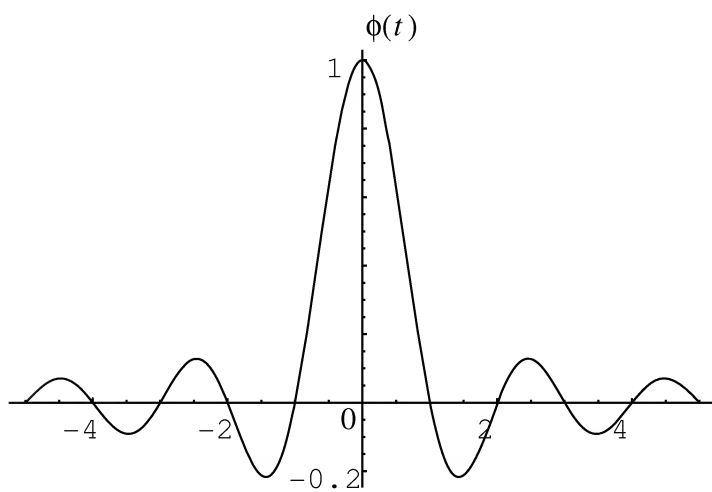
Fig. 8.3.1. Haar Family of Wavelets.



Second Generation of Haar Daughter Wavelets
Fig. 8.3.2. Haar Family of Wavelets.



Second Generations sons of the Haar Family of Wavelets
Fig. 8.3.3. Haar Family of Wavelets.

Fig. 8.3.4. Graph of $f(t)$.Fig. 8.3.5. Graph of $|\Psi(\omega)|$.Fig. 8.4.1. Shannon Wavelet $\phi(t)$.

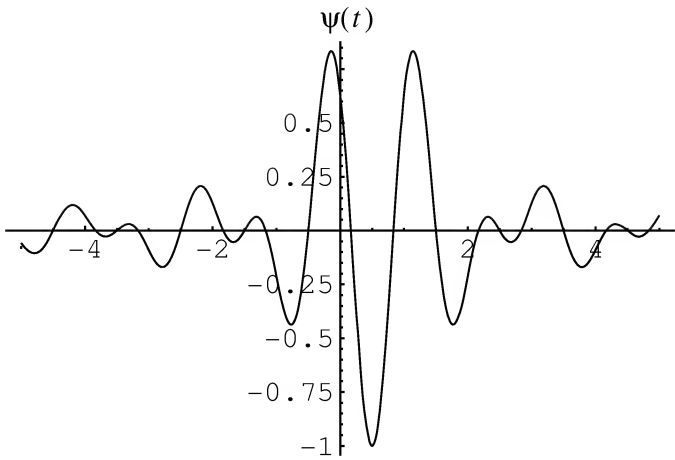


Fig. 8.4.2. Shannon Wavelet $\psi(t)$.

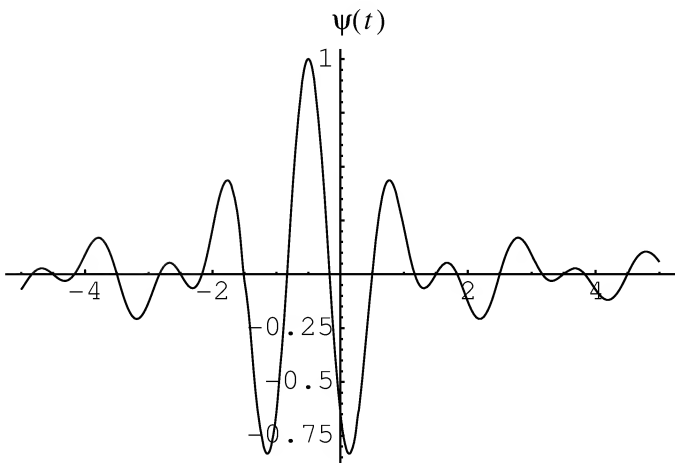


Fig. 8.4.3. Another Form of Shannon Wavelet $\psi(t)$.

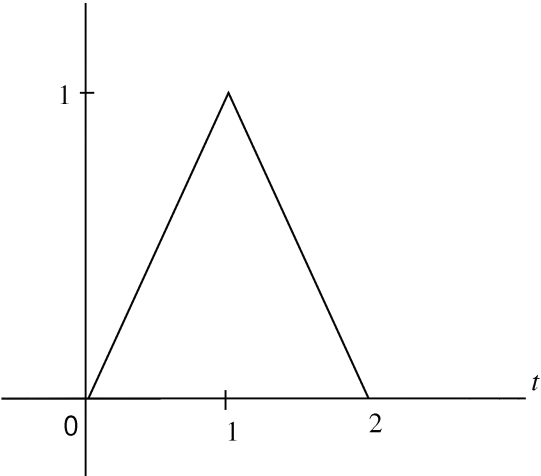


Fig. 8.4.4. Hat Wavelet.

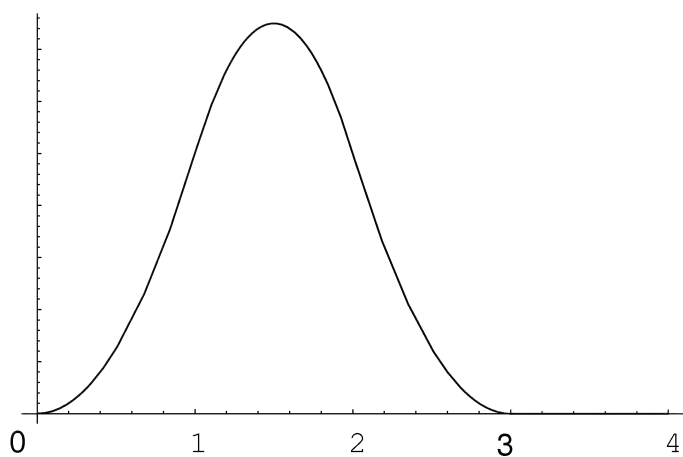
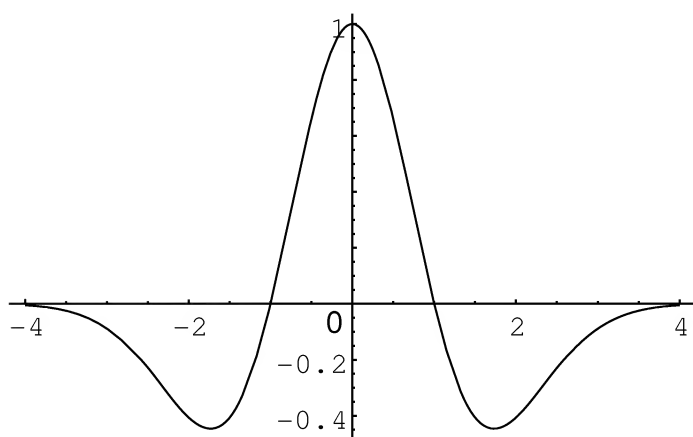
Fig. 8.4.5. Quadratic Battle-Lemarié Wavelet $\psi(t)$.

Fig. 8.4.6. Mexican Hat Wavelet.

Chapter 9

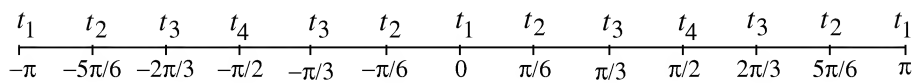


Fig. 9.3.1.

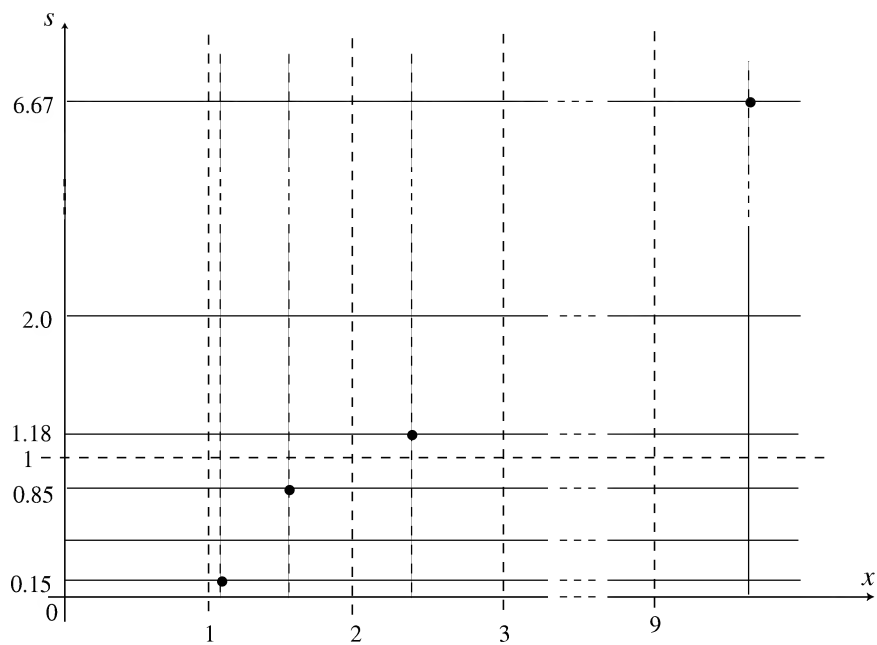


Fig. 9.4.1.

C

Contents of the CD-R

To view the .pdf files, use Acrobat Reader 5.0 or higher.

1. 38TestFunctions.pdf

2. Algorithms: algorithms.pdf

3. BitReversalAlgorithms.pdf

4. Boundary Element Method:

4.a. bem.pdf

4.b. BEMCodes DOS: Be1.c, Be2.c, Be5.c, Be11.c

4.c. BEMCodes UNIX: Be1.c, Be2.c, Be5.c, Be11.c

5. Computation Codes

5.a. f90 Codes:

aitken.f90	binocoef.f90	difftabl.f90
eps.f90	epsr.f90	eul.f90
extrpol.f90	f1.f90	f2.f90
fft.f90	fftttest.f90	fn1.f90
fn2.f90	gauleg.f90	GaussLegendre.f90
hartley2d.f90	ht.f90	ht2d.f90
inteps.f90	intepsr.f90	inteul.f90
intphi.f90	intrho.f90	intrhohat.f90
intromx.f90	intrpol.f90	neville.f90
phi.f90	rho.f90	romb.f90
ser1.f90	sub1.f90	trap.f90
trapsimp.f90	xfht.f90	

Read the file README about these codes.

Many Fortran codes for numerical quadrature, Fourier integrals and Fourier and Laplace transforms are available on the internet; others can be purchased from the ACM Transactions of Math. Software. Other resources are the NAG Ltd. (1996) and Krommer and Ueberhuber (1998).

5.b. MATLAB Codes:

adamsx.m	AdamsBashforth.m	difftabl.m
extrpol.m	fht.m	fht2d.m
GaussLegendre.m	intrpol.m	NodesWeights.m
neville.m	trapsimp.m	

MATLAB codes are available at the internet; for wavelets some websites are:

<http://liinwww.ira.uka.de>
<http://www.cosy.sbg.ac.at/~uhl/wav.html>
<http://stat.stanford.edu/~wavelab/>
<http://www.mathcad.com/products/we pack.asp?page=3>
<http://www.wavelet.org/>
<http://www.math.yale.edu/pub/wavelets/papers/acoustic.tex>.

Another source for wavelets is Misiti et al. (1997-2000).

5.c. Mathematica Codes:

bellman.nb	BracewellBunemann.nb	coeffs.nb
difftabl.nb	dirichlet1.nb	dirichlet2.nb
dirichlet3.nb	durbin.nb	error1.nb
error2.nb	error3.nb	ex2.5.1.nb
ex2.10.7.nb	ex7.4.8.nb	extrpol.nb
fht2d.nb	GaussLegendre.nb	GaussLegendreEx.nb
gaussmoments.nb	gausspts4-6.nb	gausspts12.nb
gausspts13.nb	intrpol.nb	lobatto.nb
logkernel.nb	neville.nb	nystrom1.nb
nystrom2.nb	nystrom3.nb	phillips.nb
piessens.nb	quadrature.nb	radou.nb
rhoat.nb	richard.nb	SidiNodes.nb
singular.nb	Table2.2.nb	Table2.5.nb
trapsimp.nb	tzou.nb	weeks.nb

6. CotesianNumbers.pdf

7. Figures: figures.pdf contains:

- Chapter 2: [Fig. 2.7.1](#)
 Chapter 7: [Fig. 7.5.1](#). Talbot Contours
 Chapter 8: [Fig. 8.2.1](#). Gibbs Phenomenon
[Fig. 8.3.1](#). Haar Family of Wavelets
[Fig. 8.3.2](#). Haar Family of Wavelets
[Fig. 8.3.3](#). Haar Family of Wavelets
[Fig. 8.3.4](#). Graph of $f(t)$
[Fig. 8.3.5](#). Graph of $|\Psi(\omega)|$
[Fig. 8.4.1](#). Shannon Wavelet $\phi(t)$
[Fig. 8.4.2](#). Shannon Wavelet $\psi(t)$
[Fig. 8.4.3](#). Another Form of Shannon Wavelet $\psi(t)$
[Fig. 8.4.4](#). Hat Wavelet
[Fig. 8.4.5](#). Quadratic Battle-Lemarié Wavelet $\psi(t)$

[Fig. 8.4.6. Mexican Hat Wavelet](#)

Chapter 9: [Fig. 9.3.1](#)

[Fig. 9.4.1](#)

8. Integration Formulas:

8.a. [HowTo.pdf](#)

8.b. Integration Tables: The following three sets in 8.2.1, 8.2.2 and 8.2.3 list pdf files which contain over 5,800 integration formulas. Read [HowTo.pdf](#) before using these tables.

8.b.1. Indefinite Integrals:

T1.01.pdf	T1.02.pdf	T1.03.pdf	T1.04.pdf	T1.05.pdf
T1.06.pdf	T1.07.pdf	T1.08.pdf	T1.09.pdf	T1.10.pdf
T1.11.pdf	T1.12.pdf	T1.13.pdf	T1.14.pdf	T1.15.pdf
T1.16.pdf	T1.17.pdf	T1.18.pdf	T1.19.pdf	T1.20.pdf
T1.21.pdf	T1.22.pdf	T1.23.pdf	T1.24.pdf	T1.25.pdf
T1.26.pdf	T1.27.pdf	T1.28.pdf	T1.29.pdf	T1.30.pdf
T1.31.pdf	T1.32.pdf	T1.33.pdf	T1.34.pdf	T1.35.pdf
T1.36.pdf	T1.37.pdf	T1.38.pdf		

8.b.2. Finite Range Definite Integrals:

T2.01A.pdf	T2.02A.pdf	T2.02B.pdf	T2.02C.pdf	T2.03A.pdf
T2.03B.pdf	T2.03C.pdf	T2.04A.pdf	T2.04B.pdf	T2.04C.pdf
T2.05A.pdf	T2.06A.pdf	T2.07A.pdf	T2.08A.pdf	T2.08B.pdf
T2.09A.pdf	T2.09B.pdf	T2.09C.pdf	T2.10A.pdf	T2.10B.pdf
T2.10C.pdf	T2.11A.pdf	T2.12A.pdf	T2.12B.pdf	T2.12C.pdf
T2.12D.pdf	T2.13A.pdf	T2.13B.pdf	T2.13C.pdf	T2.14A.pdf
T2.14B.pdf	T2.14C.pdf	T2.15A.pdf	T2.15B.pdf	T2.16A.pdf
T2.16B.pdf	T2.16C.pdf	T2.17A.pdf	T2.17B.pdf	T2.17C.pdf
T2.18A.pdf	T2.18B.pdf	T2.19A.pdf	T2.19B.pdf	T2.19C.pdf
T2.20A.pdf	T2.21A.pdf	T2.22A.pdf	T2.22B.pdf	T2.22C.pdf
T2.22D.pdf	T2.23A.pdf	T2.23B.pdf	T2.23C.pdf	T2.23D.pdf
T2.24A.pdf	T2.24B.pdf	T2.24C.pdf	T2.24D.pdf	T2.25A.pdf
T2.25B.pdf	T2.25C.pdf	T2.26A.pdf	T2.26B.pdf	T2.27A.pdf
T2.27B.pdf	T2.27C.pdf	T2.27D.pdf	T2.28A.pdf	T2.29A.pdf
T2.29B.pdf	T2.30A.pdf	T2.30B.pdf	T2.31A.pdf	T2.31B.pdf
T2.32A.pdf	T2.33A.pdf	T2.33B.pdf	T2.33C.pdf	T2.34A.pdf
T2.35A.pdf	T2.35B.pdf	T2.35C.pdf	T2.36A.pdf	T2.37A.pdf
T2.37B.pdf	T2.37C.pdf	T2.38A.pdf	T2.38B.pdf	T2.39A.pdf
T2.39B.pdf	T2.40A.pdf	T2.41A.pdf	T2.41B.pdf	T2.41C.pdf
T2.42A.pdf	T2.42B.pdf	T2.43A.pdf	T2.43B.pdf	T2.43C.pdf
T2.43D.pdf	T2.43E.pdf	T2.44A.pdf	T2.44B.pdf	T2.44C.pdf
T2.45A.pdf	T2.45B.pdf	T2.45C.pdf	T2.45D.pdf	T2.45E.pdf
T2.45F.pdf	T2.45G.pdf	T2.46A.pdf	T2.46B.pdf	T2.46C.pdf
T2.46D.pdf	T2.46E.pdf	T2.47A.pdf	T2.47B.pdf	T2.48A.pdf
T2.49A.pdf	T2.49B.pdf	T2.50A.pdf	T2.50B.pdf	T2.50C.pdf
T2.51A.pdf	T2.51B.pdf	T2.51C.pdf	T2.52A.pdf	T2.53A.pdf

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T2.53B.pdf	T2.53C.pdf	T2.53D.pdf	T2.53E.pdf	T2.53F.pdf
T2.54A.pdf	T2.54B.pdf	T2.54C.pdf	T2.54D.pdf	T2.54E.pdf
T2.55A.pdf	T2.55B.pdf	T2.55C.pdf	T2.56A.pdf	T2.56B.pdf
T2.56C.pdf	T2.56D.pdf	T2.56E.pdf	T2.57A.pdf	T2.57B.pdf
T2.58A.pdf	T2.58B.pdf	T2.58C.pdf	T2.59A.pdf	T2.59B.pdf
T2.60A.pdf	T2.61A.pdf	T2.62A.pdf	T2.62B.pdf	T2.63A.pdf
T2.63B.pdf	T2.63C.pdf	T2.63D.pdf	T2.63E.pdf	T2.64A.pdf
T2.64B.pdf	T2.64C.pdf	T2.65A.pdf	T2.65B.pdf	T2.66A.pdf
T2.67A.pdf	T2.67B.pdf	T2.67C.pdf	T2.68A.pdf	T2.69A.pdf
T2.69B.pdf	T2.69C.pdf	T2.69D.pdf	T2.69E.pdf	T2.69F.pdf
T2.70A.pdf	T2.71A.pdf	T2.71B.pdf	T2.72A.pdf	T2.72B.pdf
T2.72C.pdf	T2.72D.pdf	T2.72E.pdf	T2.72F.pdf	T2.73A.pdf
T2.73B.pdf	T2.74A.pdf	T2.75A.pdf	T2.75B.pdf	T2.76A.pdf
T2.76B.pdf	T2.77A.pdf	T2.78A.pdf	T2.78B.pdf	T2.79A.pdf

8.b.3. Infinite Range Definite Integrals:

T3.01A.pdf	T3.01B.pdf	T3.01C.pdf	T3.01D.pdf	T3.01E.pdf
T3.02A.pdf	T3.02B.pdf	T3.02C.pdf	T3.03A.pdf	T3.04A.pdf
T3.05A.pdf	T3.06A.pdf	T3.07A.pdf	T3.08A.pdf	T3.09A.pdf
T3.10A.pdf	T3.10B.pdf	T3.11A.pdf	T3.12A.pdf	T3.13A.pdf
T3.14A.pdf	T3.15A.pdf	T3.16A.pdf	T3.17A.pdf	T3.18A.pdf
T3.19A.pdf	T3.20A.pdf	T3.20B.pdf	T3.20C.pdf	T3.21A.pdf
T3.21B.pdf	T3.22A.pdf	T3.23A.pdf	T3.23B.pdf	T3.24A.pdf
T3.24B.pdf	T3.24C.pdf	T3.25A.pdf	T3.25B.pdf	T3.25C.pdf
T3.26A.pdf	T3.26B.pdf	T3.26C.pdf	T3.26D.pdf	T3.27A.pdf
T3.27B.pdf	T3.28A.pdf	T3.28B.pdf	T3.28C.pdf	T3.29A.pdf
T3.29B.pdf	T3.30A.pdf	T3.30B.pdf	T3.31A.pdf	T3.31B.pdf
T3.31C.pdf	T3.32A.pdf	T3.32B.pdf	T3.33A.pdf	T3.34A.pdf
T3.35A.pdf	T3.35B.pdf	T3.35C.pdf	T3.36A.pdf	T3.36B.pdf
T3.36C.pdf	T3.37A.pdf	T3.37B.pdf	T3.38A.pdf	T3.38B.pdf
T3.39A.pdf	T3.40A.pdf	T3.40B.pdf	T3.40C.pdf	T3.41A.pdf
T3.41B.pdf	T3.42A.pdf	T3.42B.pdf	T3.43A.pdf	T3.43B.pdf
T3.43C.pdf	T3.44A.pdf	T3.45A.pdf	T3.46A.pdf	T3.47A.pdf
T3.48A.pdf	T3.49A.pdf	T3.50A.pdf	T3.50B.pdf	T3.51A.pdf
T3.51B.pdf	T3.52A.pdf	T3.52B.pdf	T3.53A.pdf	T3.53B.pdf
T3.54A.pdf	T3.54B.pdf	T3.54C.pdf	T3.55A.pdf	T3.55B.pdf
T3.56A.pdf	T3.56B.pdf	T3.57A.pdf	T3.57B.pdf	T3.58A.pdf
T3.59A.pdf	T3.60A.pdf	T3.61A.pdf	T3.61B.pdf	T3.62A.pdf
T3.63A.pdf	T3.64A.pdf	T3.65A.pdf		

- 8.c. SpecialFunctions.pdf
- 8.d. TablesBiblio.pdf
- 8.e. TablesNotation.pdf

9. NewLaplaceInverses.pdf

10. Quadrature Tables: [Table A.01](#), ..., [Table A.32](#)

Bibliography

- A. ABBATE, C. M. DECUSATIS AND P. K. DAS, *Wavelets and Subbands*, Birkhäuser, Boston MA, 2002.
- J. ABDALKHANI, *A modified approach to the numerical solution of linear weakly singular Volterra integral equations of the second kind*, J. Integral Eqns. Appls., **5** (1993), 149–166.
- E. ABOUFADEL AND S. SCHLICHER, *Discovering Wavelets*, Wiley, New York, 1999.
- M. ABRAMOWITZ AND I. A. STEGUN (EDS.), *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*, National Bureau of Standards, Appl. Math. Series 55, U.S. Govt. Printing Office, Washington, DC; reprinted by Dover, New York, 1968.
- A. ALAYLIOGLU, G. A. EVANS AND J. HYSLOP, *The evaluation of integrals with infinite limits*, J. Comp. Phys., **13** (1973), 433–438.
- G. A. EVANS AND J. HYSLOP, *The use of Chebyshev series for the evaluation of oscillatory integrals*, Computer J., **19** (1976), 258–267.
- P. ALBRECHT AND G. HONIG, *Numerische Inversion der Laplace Transformierten*, Angewandte Informatik, **18** (1977), 336–345.
- T. ALFREY, *Non-homogeneous stress in viscoelastic media*, Quart. Appl. Math., **2** (1944), 113–119.
- R. S. ANDERSSSEN, F. R. DE HOGG AND M. A. LUKAS (eds.), *The Application and Numerical Solution of Integral Equations*, Sijhoff and Noordhoff International Publishers, The Netherlands, 1980.
- AND P. M. PRENTER, *A formal comparison of methods proposed for the numerical solution of first kind Fredholm equations*, J. Aust. Math. Soc., **B 22** (1981), 488–500.
- D. D. ANG, J. LIND, AND F. STENGER, *Complex variable and regularization methods of inversion of the Laplace transform*, Math. Comp., **53** (1989), 589–608.
- P. M. ANSELONE, *Nonlinear Integral Equations*, University of Wisconsin Press, Madison, 1964.
- , *Collectively Compact Operator Approximation Theory and Applications to Integral Equations*, Prentice-Hall, Englewood Cliffs, NJ, 1971.
- , *Singularity subtraction in the numerical solution of integral equations*, J. Aust. Math. Soc., **B 22** (1981), 408–418.
- AND R. H. MOORE, *Approximate solutions of integral and operator equations*, J. Math. Anal. Appls., **9** (1964), 268–277.
- H. ANTES, *Über die vierdimensionale Romberg-Integration mit Schranken*, Computing, **9** (1972), 45–52.

- P. APPELL, *Sur une classe de polynome à deux variables et le calcul approche des integrales double*, Ann. Fac. Sci., Univ. Toulouse, **4** (1890), H1–H20.
- H. ASHLEY AND M. LANDAHL, *Aerodynamics of Wings and Bodies*, Dover, New York, 1985.
- S. A. ASHOUR, *Numerical solution of integral equations with finite part integrals*, International J. Math. and Math. Scs., **22** (1999), 155.
- K. E. ATKINSON, *Extension of the Nyström method for the numerical solution of linear integral equations of the second kind*, Ph.D. Thesis, University of Wisconsin, 1966.
- , *The numerical solution of Fredholm integral equations of the second kind*, SIAM J. Numer. Anal., **4** (1967), 337–348.
- , *The numerical solution of an Abel integral equation by a product trapezoidal method*, Report, Computer Center, Australian National University, Canberra (1971).
- , *The numerical solution of Fredholm integral equations of the second kind with singular kernels*, Numer. Math., **19** (1972), 248–259.
- , *Iterative variants of the Nyström method for the numerical solution of integral equations*, Numer. Math., **22** (1973), 17–31.
- , *A Survey of Numerical Methods for the Solution of Fredholm Integrals Equations of the Second Kind*, SIAM, Philadelphia, 1976.
- , *The Numerical Treatment of Integral Equations*, Clarendon Press, Oxford, second printing, 1978.
- , *Piecewise polynomial collocation for integral equations on surfaces in three dimensions*, J. Integral Eqns., **9** (suppl.) 1985), 24–48.
- , *On the discrete Galerkin method for Fredholm integral equations of the second kind*, IMA J. Numer. Anal., **9** (1989), 385.
- , *A survey of numerical methods for solving nonlinear integral equations*, J. Integral Eqns. Appls., **4** (1992), 15.
- , *Numerical integration of line integrals*, SIAM J. Numer. Anal., **30** (1993), 882–888.
- , *The Numerical Solution of Integral Equations of the Second Kind*, Cambridge Univ. Press, Cambridge, 1997.
- AND J. FLORES, *The discrete collocation method for nonlinear integral equations*, IMA J. Numer. Anal., **13** (1993), 195.
- AND G. F. MILLER (EDS.), *Treatment of Integral Equations by Numerical Methods*, Academic Press, London, 1982.
- AND I. H. SLOAN, *The numerical solution of first-kind logarithmic-kernel integral equations on smooth open arcs*, Math. of Comput., **56** (1992), 119.
- E. E. AUBANEL AND K. B. OLDHAM, *Fourier smoothing without the fast Fourier transform*, BYTE, (February 1985), 207–218.
- F. AUGUST, *Über eine Verallgemeinerung der Gauss'schen Methode der mechanischen Quad-ratur*, Arch. f. Mathem. u. Phys., **67** (1881), 72–93.
- E. BABOLIAN AND L. M. DELVES, *An augmented Galerkin method for first kind Fredholm equations*, J. Inst. Math. Appl., **24** (1979), 157–174.
- V. A. BAKALETS AND N. P. GRITSYUK, *Two numerical methods for solving integral equations with a weak singularity*, J. Soviet Math., **58** (1992), 202.
- C. T. H. BAKER, *On the nature of certain quadrature formulas and their errors*, J. Numer. Anal., **5** (1968), 783–804.
- , *The Numerical Treatment of Integral Equations*, Clarendon Press, Oxford, second printing, 1978.
- , *An introduction to the numerical treatment of Volterra and Abel-type integral equations*, in Topics in Numerical Analysis (P. R. Turner, ed.), Lecture Notes in Mathematics #965, Springer-Verlag, Berlin, 1982, pp. 1–35.
- C. T. H. BAKER AND M. S. DERAKSHAN, *Fast generation of quadrature rules with some special properties*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 53–60.

- , L. FOX, D. F. MAYERS AND K. WRIGHT, *Numerical solution of Fredholm integral equations of first kind*, Computer J., **7** (1964), 141–148.
- AND G. F. MILLER (EDS.), *Treatment of Integral Equations by Numerical Methods*, Academic Press, London, 1982.
- N. S. BAKHNALOV AND L. G. VASILEVA, *Evaluation of the integrals of oscillating functions by interpolation at nodes of Gaussian quadratures*, Z. Vycisl. mat. i mat. fiz., **8** (1968), 175–181. (Russian)
- G. BALBINE AND J. N. FRANKLIN, *The calculation of Fourier integrals*, Math. Comp., **20** (1960), 570–589.
- R. BALIAN, *Un principe d'incertitude fort en théorie du signal ou en mécanique quantique*, C. R. Acad. Sci. Paris, **292**, (Série II, 1981), 1357–1361.
- N. S. BAKHVALOV AND L. G. VASIL'eva, *Evaluation of the integrals of oscillating functions by interpolation at nodes of Gaussian quadratures*, SSSR Comp. Math. Phys., **8** (1968), 241–249.
- N. K. BASU, *Error estimates for a Chebyshev quadrature method*, Math. Comp., **24** (1970), 863–867.
- H. BATEMAN, *Two systems of polynomials for the solution of Laplace's integral equation*, Duke Math. J., **2** (1936), 569–577.
- F. L. BAUER, H. RUTISHAUSER AND E. STIEFEL, *New aspects in numerical quadrature*, Proc. Symposia in Appl. Math., Amer. Math. Soc., Providence (1963), 199–219.
- R. E. BEARD, *Some notes on approximate product integration*, J. Inst. Actu., **73** (1947), 356–416.
- J. A. BELWARD, *The solution of an integral equation of the first kind on a finite interval*, Quart. Appl. Math., **27** (1969), 313–321.
- , *Further studies of the application of constrained minimization methods to Fredholm integral equations of the first kind*, IMA J. Numer. Anal., **5** (1985), 125–139.
- D. A. BELL, *Approximations in Fourier transforms*, Comput. J., **6** (1963–1964), 244–247.
- R. BELLMAN, H. KAGIWADA AND R. E. KALABA, *Identification of linear systems via numerical inversion of Laplace transforms*, IEEE Trans. Automatic Control, **AC-10** (1965), 111–112.
- , R. E. KALABA AND J. A. LOCKETT, *Numerical Inversion of the Laplace Transform: Applications to Biology, Economics, Engineering and Physics*, American Elsevier, New York, 1966.
- I. S. BEREZIN AND N. P. ZHIDKOV, *Computing Methods*, vol. 1, Addison–Wesley, Reading, MA, and Pergamon Press, Oxford, UK, 1965. (Russian)
- B. S. BERGER, *Tables of Zeros and Weights for Gauss–Legendre quadrature to 23–24S for $n = 100, 150, 200(100)900$* , Dept. of Mech. Eng., Univ. of Maryland, College Park, MD, 1969a.
- , *Tables of Zeros and Weights for Gauss–Hermite quadrature to 26–27S for $n = 200(200)1000, 2000$* , Dept. of Mech. Eng., Univ. of Maryland, College Park, MD, 1969b.
- J. BERNTSEN AND T. O. ESPELID, *Error estimation in automatic quadrature routines*, ACM Trans. Math. Software, **17** (1991a), 233–252.
- , T. O. ESPELID AND T. SOEREVERIK, *On the subdivision strategy in adaptive quadrature algorithms*, J. Comp. Appl. Math., **35** (1991b), 119–132.
- S. N. BERNSTEIN, *On quadrature formulas of Cotes and Tschebyscheff*, Doklady Akad. Nauk SSSR, **14** (1937), 323–326. (Russian)
- B. BERTRAM, *Numerical implementation of a Brakhage-like technique for weakly singular integral equations using product integration*, Computers & Math. with Applications, **26** (1993), 21.
- AND O. RUEHR, *Product integration for finite-part singular integral equations: numerical asymptotics and convergence acceleration*, J. Comput. Appl. Math., **41** (1992), 163.
- W. H. BEYER, *CRC Standard Mathematical Tables*, CRC Press, Boca Raton, FL, 1986.

- B. BIALECKI, *A modified sinc quadrature rule for functions with poles near the arc of integration*, BIT, **29** (1989), 464–476.
- , *A sinc-Hunter quadrature rule for Cauchy principal value integrals*, Math. Comp., **55** (1990), 665–681.
- , *A sinc quadrature rule for Hadamard finite part integrals*, Numer. Math., **75** (1990), 263–269.
- , *Sinc quadrature for Cauchy principal value integrals*, in Numerical Integration — Recent Developments, Software and Applications (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 81–92.
- C. BLATTER, *Wavelets: A Primer*, A. K. Peters, Natick MA, 1998.
- N. BLEISTEIN AND R. A. HANDELSMAN, *Asymptotic Expansions of Integrals*, Holt, Rinehart and Winston, New York, 1975.
- J. L. BLUE, *Automatic numerical quadrature — DQUAD*, Computer Sc. Tech. Rep. 25 (1975), Bell Labs., Murray Hill, NJ.
- , *Automatic numerical quadrature*, Bell System Tech. J., **56** (1977), 1651–1678.
- W. B. BICKFORD, *A First Course in the Finite Element Method*, Irwin, Boston, MA, 1990.
- R. P. BOAS, JR. AND D. V. WIDDER, *An inversion formula for the Laplace integral*, Duke Math. J., **6** (1940), 1–26.
- W. R. BOLAND, *The convergence of product-type quadrature formulas*, SIAM J. Numer. Anal., **9** (1972), 6–13.
- , *The numerical solution of Fredholm integral equations using product-type quadrature formulas*, BIT, **12** (1972a), 5–16.
- , *Algorithm 436. Product type trapezoidal integration*, Comm. ACM, **15** (1972b), 1070.
- , *Algorithm 437. Product type Simpson's integration*, Comm. ACM, **15** (1972c), 1071.
- , *Algorithm 438. Product type two-point Gauss-Legendre-Simpson's integration*, Comm. ACM, **15** (1972d), 1071.
- , *Algorithm 439. Product type three-point Gauss-Legendre-Simpson's integration*, Comm. ACM, **15** (1972e), 1072.
- , *Properties of product-type quadrature formulas*, BIT, **13** (1973), 287–291.
- B. A. BOLEY AND C. C. CHAO, *Some solutions of the Timoshenko beam equations*, J. Appl. Mech., **22** (1955), 579–586.
- J. P. BORIS AND E. S. ORAN, *Numerical evaluation of oscillatory integrals such as the modified Bessel function $K_{i\xi}(x)$* , J. Comp. Phys., **17** (1975), 425–433.
- G. BOROS AND V. H. MOLL, *An integral with three parameters*, SIAM Rev., **40** (1998), 972–980.
- AND V. H. MOLL, *An integral hidden in Gradshteyn and Ryzhik*, J. Comput. Appl. Math., **106** (1999), 361–368.
- AND V. H. MOLL, *A sequence of unimodal polynomials*, J. Math. Anal. Appl., **237** (1999), 272–287.
- AND V. H. MOLL, *The double square root, Jacobi polynomials and Ramanujan's Master Theorem*, J. Comput. Appl. Math., **130** (2001), 337–344.
- AND V. H. MOLL, *Landen transformations and the integration of rational functions*, Math. Comput., **71** (238) (2002), 649–668.
- , O. ESPINOSA AND V. H. MOLL, *On some families of integrals solvable in terms of polygamma and negapolygamma functions*, Integr. Transf. Spec., **14** (3) (2003), 187–203.
- J.-P. BOUJOT AND P. MARONI, *Algorithme général de construction de tables de Gauss pour les problèmes de quadratures*, Publ. No. MMX/8.1.8/AI. Inst. Blaise Pascal, Paris, 1968.
- R. N. BRACEWELL, *The discrete Hartley transform*, J. Optical Soc. of America, **73** (1983), 1832.

- , *The Hartley Transform*, Oxford University Press, New York, 1986.
- H. BRAKHAGE, *Über die numerische Behandlung von Integralgleichungen nach der Quadrature Formelmethode*, Numer. Math., **2** (1960), 183–196.
- M. BRANDERS AND R. PIESENS, *Algorithm 001: An extension of Clenshaw-Curtis quadrature*, J. Comp. Appl. Math., **1** (1965), 55–65.
- R. PIESENS, *Algorithm 1: An extension of Clenshaw-Curtis quadrature*, J. Comp. Appl. Math., **1** (1975), 55–65.
- H. BRASS (BRAß), *Quadraturverfahren*, Vandenhoeck und Ruprecht, Göttingen, 1977.
- C. BREZINSKI, *A subroutine for the general interpolation and extrapolation problems*, ACM Trans. Math. Software, **8** (1982), 290–301.
- J. BRONSTEIN, *Integration of elementary functions*, J. Symbol. Comput., **9** (1990), 117–173.
- , *Symbolic Integration I — Transcendental Functions*, Springer-Verlag, Berlin, 1996, pp. 117–173.
- R. BROUCKE, *Algorithm 446: Ten subroutines for the manipulation of Chebyshev series*, Comm. ACM, **16** (1973), 254–256.
- T. A. BROWN, *Fourier's integral*, Proc. Edinburgh Math. Soc., **34** (1915–1916), 3–10.
- R. BULIRSCH, *Bemerkungen zur Romberg integration*, Num. Math., **6** (1964), 1–13.
- AND J. STOER, *Numerical quadrature by extrapolation*, Num. Math., **9** (1967), 271–278.
- O. BUNEMAN, *Conversion of FFT's to fast Hartley transforms*, SIAM J. Sci. Stat. Comput., **7** (1986), 624–638.
- R. S. BURINGTON (ed.), *Handbook of Mathematical Tables and Formulas*, McGraw-Hill, New York, 1962.
- J. S. BYRNES (ed.), *Wavelets and Their Applications*, Kluwer Academic Publisher, 1994.
- D.-W. BYUN AND S. SAITOH, *A real inversion formula for the Laplace transform*, Zeitschrift für Analysis und ihre Anwendungen, **12** (1993), 597–603.
- A. P. CALDERÓN, *An atomic decomposition of distributions in parabolic H^p spaces*, Advances in Math., **25** (1978), 85–96.
- J. CALDWELL, *Numerical study of Fredholm integral equations*, Intl. J. Math. Educ., **25** (1994), 831–836.
- F. CALIO AND E. MARCHETTI, *Derivation and implementation of an algorithm for singular integrands*, Computing, **38** (1987), 235–245.
- AND E. MARCHETTI, *Complex Gauss-Kronrod integration rules for certain Cauchy principal value integrals*, Computing, **50** (1993), 165–173.
- T. CAO, *Hierarchical basis methods for hypersingular integral equations*, IMA J. Numer. Anal., **17** (1997), 603.
- O. CARINO, I. ROBINSON AND E. DE DONCKER, *An algebraic study of the Levin transform in numerical integration*, in Numerical Integration — Recent Developments, Software and Applications (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 175–186.
- G. F. CARRIER, M. KROOK AND C. E. PEARSON, *Functions of a Complex Variable*, McGraw-Hill, New York, 1966.
- C. CARSTENSEN AND E. P. STEPHAN, *Adaptive boundary element methods for some first kind integral equations*, SIAM J. Numer. Anal., **33** (1996), 2166.
- J. CASSALETTO, M. PICKET AND J. R. RICE, *A comparison of some integration programs*, SIGNUM Newsletter, **4** (1969), 30–40.
- J. L. CASTI, *A family of Fredholm integral equations*, Problem 72-2, SIAM Rev., **15** (1973), 220–221.
- , R. KALABA AND S. UENO, *Cauchy systems for Fredholm integral equations with parameter imbedding*, Appl. Math. Comput., **108** (2000), 47.
- LL. G. CHAMBERS, *Integral Equations. A Short Course*, International Textbook Co. Ltd., London, 1976.
- S. M. CHASE AND L. D. FOSDICK, *An algorithm for Filon quadrature*, Comm. ACM, **12** (1969), 453–457.

- M. M. CHAWLA, *On the Chebyshev polynomials of the second kind*, SIAM Rev., **9** (1967), 729–733.
- , *Convergence of Newton-Cotes quadratures for analytic functions*, BIT, **11** (1971), 159–167.
- AND S. KUMAR, *Convergence of quadratures for Cauchy principal value integrals*, Computing, **23** (1979), 67–72.
- P. L. CHEBYCHEV, *On quadratures*, J. Math. Pures Appl., (2), **19** (1874), 19–34.
- T. H. C. CHEN, *Asymptotic error estimates for Gaussian quadrature formulas*, Math. Comp., **38** (1982), 143–152.
- E. W. CHENEY, *Introduction to Approximation Theory*, McGraw-Hill, New York, 1966.
- G. W. CHERRY, *Integration in finite terms with special functions: The logarithmic integral*, SIAM J. Comput., **15** (1986), 1–21.
- C. CHIARELLA AND A. REICHEL, *On the evaluation of integrals related to the error function*, Math. Comp., **22** (1968), 137–143.
- C. CHIDO AND G. CRISCUOLO, *On the convergence of a rule by Monegato for the numerical evaluation of Cauchy principal value integrals*, Computing, **40** (1988), 67–74.
- J. S. R. CHISHOLM, A. GENZ AND G. E. ROWLANDS, *Accelerated convergence of sequences*, J. Comp. Phys., **10** (1972), 284–307.
- E. B. CHRISTOFFEL, *Über die Gaussische Quadratur und eine Verallgemeinerung derselben*, J. Reine Angew. Math., **55** (1858), 61–82.
- A. C. CHRYSAKIS AND G. TSAMASPHYROS, *Numerical solution of Cauchy type singular integral equations with logarithmic weight, based on arbitrary collocation points*, Comput. Mech., **7** (1990), 21.
- AND G. TSAMASPHYROS, *Numerical solution of integral equations with a logarithmic kernel by the method of arbitrary collocation points*, Intl. J. Numer. Methods in Elasticity, **33** (1992), 143.
- C. K. CHUI, *An Introduction to Wavelets*, Academic Press, 1992.
- , *Wavelets: A Mathematical Tool for Signal Analysis*, SIAM, Philadelphia, 1997.
- W. W. CLENDENIN, *A method for numerical calculation of Fourier integrals*, Numer. Math., **8** (1966), 422–436.
- C. W. CLENSHAW, *The numerical solution of linear differential equations in Chebyshev series*, Proc. Camb. Phil. Soc., **53** (1957), 134–149.
- , *Chebyshev series for mathematical functions*, Math. Tables, **5** (1962), National Physical Laboratory, London: H.M.S.O..
- AND A. R. CURTIS, *A method for numerical integration on an automatic computer*, Numer. Math., **12** (1960), 197–205.
- J. A. COCHRAN, *An Analysis of Linear Integral Equations*, McGraw-Hill, New York, 1972.
- A. M. COHEN, *Cautious Romberg extrapolation*, Int. J. Comp. Math., **8** (1980), 137–147.
- R. COIFMAN, *A real variable characterization of H^p* , Studia Mat., **51** (1974).
- AND Y. MEYER, *Remarques sur l'analyse de Fourier à fenêtre*, C. R. Acad. Sci. Paris Sér. I (1991a), 259–261.
- AND Y. MEYER, *Ondelettes et Opérateurs III: Opérateurs Multilinéaires*, Hermann, Paris, 1991b.
- Y. MEYER AND V. WICKERHAUSER, *Size properties of wavelet packets*, in Wavelets and Their Applications (M. B. Ruskai, G. Beylkin, R. Coifman, I. Daubechies, S. Mallat, Y. Meyer, L. Raphael, eds.), Jones & Bartlett, Boston, MA, 1992, pp. 453–470.
- AND G. WEISS, *Review of Littlewood-Paley and multiplier theory*, Bull. Amer. Math. Soc., **84** (1977a), 242–250.
- T. F. COLEMAN AND C. VANLOAN, *Handbook for Matrix Computations*, SIAM, Philadelphia, PA, 1988.
- S. D. CONTE AND C. DE BOOR, *Elementary Numerical Analysis*, 2nd ed., McGraw-Hill, New York, 1972.
- J. W. COOLEY AND J. W. TUKEY, *An algorithm for the machine calculation of complex*

- Fourier series*, Math. Comput., **19** (1965), 297–301.
- , P. A. W. LEWIS AND P. D. WELCH, *The fast Fourier transform and its applications*, IEEE Trans. Educ. E-12, **1** (1969), 27–34.
- , P. A. W. LEWIS AND P. D. WELCH, *The fast Fourier transform algorithm: Programming considerations in the calculation of sine, cosine and Laplace transforms*, J. Sound Vib., **12** (1970), 315–337.
- D. K. COPE, *Convergence of Piessens' method for numerical inversion of the Laplace transform on the real line*, SIAM J. Numer. Anal., **27** (1990), 1345–1354.
- G. F. CORLISS, *Performance of self-validating adaptive quadrature*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 239–259.
- AND G. KRENZ, *Indefinite integration with validation*, ACM Trans. Math. Software, **15** (1989), 375–393.
- T. L. COST, *Approximate Laplace transform inversions in viscoelastic stress analysis*, AIAA Journal, **2** (1964), 2157–2166.
- R. CRANLEY AND T. N. L. PATTERSON, *On the automatic numerical evaluation of definite integrals*, Math. Comput., **14** (1971), 189–198.
- G. CRISCUOLO AND G. MASTROIANNI, *On the convergence of an interpolatory product rule for evaluating Cauchy principal value integrals*, Math. Comp., **48** (1987), 725–735.
- AND G. MASTROIANNI, *On the convergence of an interpolatory product rule for the evaluation of derivatives of Cauchy principal value integrals*, SIAM J. Numer. Anal., **25** (1988), 713–727.
- AND G. MASTROIANNI, *On the uniform convergence of Gaussian quadrature rules for Cauchy principal value integrals*, Numer. Math., **54** (1989), 445–461.
- K. S. CRUMP, *Numerical inversion of Laplace transforms using a Fourier series approximation*, J. Assoc. Comp. Mach., **23** (1976), 89–96.
- A. D'ALESSIO, L. A. AMORE AND G. LACCETTI, *An effective discretization error estimate of Fourier series methods for the numerical inversion of the Laplace transform*, Recherche di Matem., **43** (1994), 293–307.
- L. D'AMORE, G. LACCETTI AND A. MURLI, *An implementation of a Fourier series method for the numerical inversion of the Laplace transform*, ACM Trans. Math. Software, **25** (1999a), 279–305.
- , G. LACCETTI AND A. MURLI, *Algorithm 796: A Fortran Software Package for the Numerical Inversion of the Laplace Transform*, ACM Trans. Math. Software, **25** (1999b), 306–315.
- C. DAGNINO, *Extended product integration rules*, BIT, **15** (1983), 488–499.
- AND C. FIORENTINO, *Computation of nodes and weights of extended Gaussian rules*, Computing, **32** (1984), 271–278.
- AND A. PALAMARA-ORSI, *Product integration of piecewise continuous integrands based on cubic spline interpolation at equally spaced nodes*, Numer. Math., **52** (1988), 459–466.
- , *Extensions of some results for interpolatory product integration rules to rules not necessarily of interpolatory type*, SIAM J. Numer. Anal., **23** (1986), 1284–1289.
- , *Product integration of singular integrands based on cubic spline interpolation at equally spaced nodes*, Numer. Math., **57** (1990), 97–104.
- AND E. SANTI, *On the evaluation of one-dimensional Cauchy principal value integrals by rules based on cubic spline nodes*, Computing, **43** (1990), 267–276.
- AND E. SANTI, *On the convergence of spline product quadratures for Cauchy principal value integrals*, J. Comput. Appl. Math., **36** (1991), 181–187.
- , V. DEMICHELIS AND E. SANTI, *An algorithm for numerical integration based on quasi-interpolating splines*, Numer. Algorithms, **5** (1993), 443–452.
- , V. DEMICHELIS AND E. SANTI, *Numerical integration based on quasi-interpolating splines*, Computing, **50** (1993), 149–163.

- I. DAUBECHIES, *Orthonormal basis of compactly supported wavelets*, Comm. Pure Appl. Math., **41** (1988), 996.
- , *The wavelet transform, time-frequency localization and signal analysis*, IEEE Trans. Inform. Theory, **36** (1990), 961–1005.
- , *Ten Lectures on Wavelets*, CBS-NSF Regional Conf. in Appl. Math., 61, SIAM, 1992.
- , A. GROSSMAN AND Y. MEYER, *Painless nonorthogonal expansions*, J. Math. Phys., **27** (1986), 1271–1283.
- , S. JAFFARD AND J. L. JOURNÉ, *A simple Wilson orthonormal basis with exponential decay*, SIAM J. Math. Anal., **22** (1991), 554–572.
- , S. MALLAT AND A. S. WILLSKY (eds.), *Special issue on wavelet transforms and multiresolution signal analysis*, IEEE Trans. Inform. Theory, **38** (1992).
- AND J. LAGARIAS, *Two scale-difference equations, I, Existence and global regularity of solution*, SIAM J. Math. Anal., **22** (1991), 1388–1410.
- AND J. LAGARIAS, *Two scale-difference equations, II, Local regularity, infinite products of matrices and fractals*, SIAM J. Math. Anal., **23** (1992), 1031–1079.
- J. H. DAVENPORT, *On the Integration of Algebraic Functions*, Lecture Notes in Computer Science, #102, Springer-Verlag, Berlin, 1981.
- B. DAVIES, *Integral Transforms and Their Applications*, Springer-Verlag, New York, 1978.
- AND B. MARTIN, *Numerical inversion of the Laplace transform: A survey and comparison of methods*, J. Comput. Phys., **33** (1979), 1–32.
- P. J. DAVIS, *On the numerical integration of periodic analytic functions*, in On Numerical Approximation (R. Langer, eds.), Univ. of Wisconsin Press, Madison, MI, 1959, pp. 45–59.
- , *Error of numerical approximation for analytic functions*, in Survey of Numerical Analysis (R. E. Langer, ed.), The University of Wisconsin press, Madison, WI, 1962, pp. 45–60.
- , *A construction of nonnegative approximate quadratures*, Math. Comp., **21** (1967), 578–582.
- , *Interpolation and Approximation*, Blaisdell, New York, 1963; Dover, New York, 1976.
- , *A construction of nonnegative approximate quadratures*, Math. Comput., **21** (1967), 578–582.
- AND P. RABINOWITZ, *Numerical Integration*, Ginn (Blaidell), Boston, MA, 1967.
- AND P. RABINOWITZ, *Methods of Numerical Integration*, 2nd ed., Academic Press, New York, 1984.
- C. DE BOOR, *On writing an automatic integration algorithm*, in Mathematical Software (J. R. Rice, ed.), Academic Press, New York, 1971a.
- , CADRE: *An algorithm for numerical quadrature*, in Mathematical Software (J. R. Rice, eds.), Academic Press, New York, 1971b, pp. 417–449.
- , *A Practical Guide to Splines*, Appl. Math. Scs., Vol. 27, Springer-Verlag, New York, 1978.
- , *Good approximation by spline with variable knots*, in Spline Functions and Approximation Theory, Birkhäuser, Basel, 1973.
- AND A. RON, *On multivariate polynomial interpolation*, Constr. Approx., **6** (1990), 287–302.
- AND A. RON, *The least solution for the polynomial interpolation problem*, Math. Z., **210** (1992), 347–378.
- E. DE DONCKER, *Asymptotic expansions and their application in numerical integration*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 141–151.
- AND R. PIESSENS, *A bibliography on automatic integration*, J. Comput. App. Math., **2** (1976a), 273–280.

- AND R. PIESSENS, *Algorithm 32. Automatic computation of integrals with singular integrand, over a finite or infinite range*, Computing, **17** (1976b), 265–279.
- AND I. ROBINSON, *An algorithm for automatic integration over a triangle using non-linear extrapolation*, ACM Trans. Math. Software, **10** (1984), 1–16.
- F. R. DE HOOG AND R. WEISS, *On the solution of Volterra integral equations of the first kind*, Numer. Math., **21** (1973a), 22–32.
- , *Asymptotic expansions for product integration*, Math. Comput., **27** (1973b), 295–306.
- , J. H. KNIGHT AND A. N. STOKES, *An improved method for numerical inversion of Laplace transforms*, SIAM J. Sci. Comput., **3** (1982), 357–366.
- J. H. DE KLERK, *Solution of integral equations via L_1 -approximations*, Intl. J. Control, **48** (1988), 2121–2128.
- , *The sensitivity of a computational L_1 -approximation technique in integral equations*, Appl. Math. Comput., **62** (1994), 171–182.
- , D. EYRE AND L. M. VERNER, *L_p -Approximation method for the numerical solution of singular integral equations*, Appl. Math. Comput., **72** (1995), 285–300.
- D. DELBOURGO AND D. ELLIOTT, *On the approximate evaluation of Hadamard finite-part integrals*, IMA J. Numer. Anal., **14** (1994), 485–500.
- L. M. DELVES, *A fast method for the solution of integral equations*, J. Inst. Math. Appl., **20** (1977), 173–182.
- AND L. P. ABD-ELAL, *Algorithm 97. The fast Galerkin algorithm for the solution of linear Fredholm equations*, Comput. J., **20** (1977), 374–376.
- AND J. WALSH (EDS.), *Numerical Solution of Integral Equations*, Clarendon Press, Oxford, 1974.
- AND J. L. MOHAMED, *Computational Methods for Integral Equations*, Cambridge University Press, Cambridge, 1985.
- AND L. F. ABD-ELAL, *Algorithm 97. The fast Galerkin algorithm for the solution of linear Fredholm equations*, Comput. J., **20** (1977), 374–376.
- , L. F. ABD-ELAL AND J. A. HENDRY, *A fast Galerkin algorithm for singular integral equations*, J. Inst. Math. Appl., **23** (1979), 139–166.
- , L. F. ABD-ELAL AND J. A. HENDRY, *A set of modules for the solution of integral equations*, Comput. J., **24** (1981), 184–190.
- A. M. DENISOV AND A. S. KRYLOV, *Numerical solution of integral equations of the first kind*, Comput. Math. and Modeling, **1** (1990), 137.
- P. DIERCK AND R. PIESSENS, *Calculation of Fourier coefficients of discrete functions using cubic splines*, J. Comput. Appl. Math., **3** (1977), 207–209.
- K. DIETHELM, *Modified compound quadrature rules for strongly singular integrals*, Computing, **52** (1994), 337–354.
- B. DIETMAR AND P. JUNGHANS, *New error bounds for the quadrature method for the solution of Cauchy singular integral equations*, SIAM J. Numer. Anal., **30** (1993), 1351.
- V. DIXON, *Bibliography*, in Software for Numerical Mathematics (D. J. Evans, ed.), Academic Press, New York, 1974, pp. 105–137.
- M. L. DOW AND D. ELLIOTT, *The numerical solution of singular integral equations over $[-1, 1]$* , SIAM J. Numer. Anal., **16** (1979).
- H. DUBNER AND J. ABATE, *Numerical inversion of Laplace transforms by relating them to the finite Fourier cosine transform*, J. Assoc. Comp. Mach., **15** (1968), 115–123.
- D. G. DUFFY, *On the numerical inversion of Laplace transforms: A survey of three new methods on characteristic problems from applications*, ACM Trans. Math. Software, **19** (1993), 333–359.
- F. DUBBIN, *Numerical inversion of Laplace transforms: An efficient improvement to Dubner and Abate's method*, The Computer J., **17** (1974), 371–376.
- C. S. DURIS, *A simplex sufficiency condition for quadrature formulas*, Math. Comp., **20**

- (1966), 68–78.
- , *Optimal quadrature formulas using generalized inverses. Pt. I. General theory and minimum variance formulas*, Math. Comp., **25** (1971), 495–504.
- , *The (q, r) copy of product-type Newton-Cotes quadrature formulas*, Math. Rep. (1974), Drexel University, Philadelphia.
- P. P. B. EGGERMONT AND CH. LUBICH, *Fast numerical solution of singular integral equations*, J. Integral Eqns. Appls., **6** (1994), 335.
- U. T. EHRENMARK, *A three-point formula for numerical quadrature of oscillatory integrals with variable frequency*, J. Comput. Appl. Math., **21** (1988), 87–99.
- B. EINARSSON, *Algorithm 418. Calculation of Fourier integrals*, Comm. ACM, **15** (1972), 47–48.
- S. E. EL-GENDI, *Chebyshev solution of differential, integral and integro-differential equations*, Comput. J., **12** (1969), 282–287.
- D. ELLIOTT, *A Chebyshev series method for the numerical solution of Fredholm integral equations*, Comput. J. **6** (1963), 102–111.
- , *Truncation errors in two Chebyshev series approximations*, Math. Comp., **19** (1965), 234–248.
- , *A Chebyshev series method for the numerical solution of Fredholm integral equations*, Comput. J., **6** (1963), 102–111.
- AND W. G. WARNE, *An algorithm for the numerical solution of linear integral equations*, ICC Bull. (Intl. Comput. Cent.), **6** (1967), 207–224.
- AND D. F. PAGET, *On the convergence of a quadrature rule for evaluating certain Cauchy principal value integrals*, Numer. Math., **23** (1975), 311–319.
- AND D. F. PAGET, *On the convergence of a quadrature rule for evaluating certain Cauchy principal value integrals — An addendum*, Numer. Math., **25** (1976), 287–289.
- AND D. F. PAGET, *Product-integration rules and their convergence*, BIT, **16** (1976), 32–40.
- AND D. F. PAGET, *Convergence of product integration rules*, BIT, **18** (1978), 137–141.
- AND D. F. PAGET, *Gauss type quadrature rules for Cauchy principal value integrals*, Math. Comp., **33** (1979), 301–309.
- AND D. F. PAGET, *Gauss type quadrature rules for Cauchy principal value integrals*, Math. Comp., **33** (1979), 301–309.
- , *The convergence of product integration rules*, BIT, **18** (1978), 137–141.
- , *An asymptotic analysis of two algorithms for certain Hadamard finite-part integrals*, IMA J. Numer. Anal., **13** (1993), 445–462.
- H. ENGELS, *Eine Zusammenstellung von Arbeiten über numerische Quadratur und Kubatur*, Report, Jül-Bibl., **16** (1972), Nuclear Res. Centre, Jülich.
- , *Numerical Quadrature and Cubature*, Academic Press, London, 1980.
- A. ERDÉLYI, *Inversion formulae for the Laplace transformation*, Phil. Mag., **34** (1943a), 533–537.
- , *Note on an inversion formula for the Laplace transformation*, J. London Math. Soc., **18** (1943b), 72–77.
- (ed.), *Tables of Laplace transforms. Bateman Manuscripts Project, Vol. I*, McGraw-Hill, New York, 1954.
- , *Asymptotic representations of Fourier integrals and the method of stationary phase*, J. SIAM, **3** (1955), 17–27.
- , *An integral equation involving Legendre's polynomial.*, Amer. Math. Monthly, **70** (1963), 651–652.
- , *An integral equation involving Legendre functions*, J. Soc. Industr. Appl. Math., **12** (1964), 15–30.
- , *Some integral equations involving finite parts of divergent integrals*, Glasgow Math. J., **8** (1967), 50–54.
- , W. MAGNUS, F. OBERHETTINGER, AND F. G. TRICOMI, *Higher Transcendental*

- Functions*, Vol. II, McGraw-Hill, New York, 1953.
- F. ERDOGAN AND G. D. GUPTA, *On the numerical solution of singular integral equations*, Quart. Appl. Math., **30** (1972), 525.
- , G. D. GUPTA AND T. S. COOK, *Numerical solution of singular integral equations*, in *Methods of Analysis and Solution of Crack Problems* (G. C. Sih, ed.), Mechanics of Fracture, Vol. 1, Noordhoff, Leyden, 1973, pp. 368–425.
- W. ESSAH, L. M. DELVES, AND J. BELWARD, *A cross validation Galerkin algorithm for first kind integral equations*, Preprint (1986), Dept. of Statistics and Computational Mathematics, University of Liverpool.
- AND L. M. DELVES, *The numerical solution of first kind integral equations*, J. Comput. Appl. Math., **27** (1989), 363–387.
- T. O. ESPELID, *On the construction of good symmetric integration rules*, SIAM J. Numer. Anal., **24** (1987), 855–881.
- AND T. SOEREBIK, *A discussion of a new error estimate for adaptive quadrature*, BIT, **29** (1989), 283–294.
- T. O. ESPELID, DQAIN: *An algorithm for adaptive quadrature (of a vector function) over a collection of finite intervals*, in *Numerical Integration — Recent Developments, Software and Applications* (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 341–342.
- AND A. GENZ (eds.), *Numerical Integration — Recent Developments, Software and Applications*, Kluwer, Dordrecht, 1992.
- , *On integrating vertex singularities using extrapolation*, BIT, **34** (1994), 62–79.
- AND K. J. OVERHOLT, DQAINF: *An algorithm for automatic integration of infinite oscillating tails*, Numer. Algorithms, **8** (1994), 83–101.
- W. ESSAH, L. M. DELVES, AND J. BELWARD, *A cross validation Galerkin algorithm for first kind integral equations*, Preprint (1986), Dept. of Statistics and Computational Mathematics, University of Liverpool.
- AND L. M. DELVES, *The numerical solution of first kind integral equations*, J. Comput. Appl. Math., **27** (1989), 363–387.
- G. A. EVANS, *Integrating oscillatory integrands of a non-trigonometric type over a finite range*, Int. J. Comp. Math., **42** (1992), 213–221.
- , *Practical Numerical Integration*, Wiley, Chichester, UK, 1993.
- , *Two robust methods for irregular oscillatory integrals over a finite range*, Appl. Numer. Math., **14** (1994), 383–395.
- G. A. EVANS, R. C. FORBES, AND J. HYSLOP, *Polynomial transformations for singular integrals*, Intl. J. Computer Math., **14** (1983), 157–170.
- J. HYSLOP AND A. P. G. MORGAN, *An extrapolation procedure for the evaluation of singular integrals*, Int. J. Comp. Math., **12** (1983), 251–265.
- G. FAIRWEATHER, *Algorithm 351. Modified Romberg quadrature*, Comm. ACM, **12** (1969), 324–325.
- P. FAVATI, G. LOTTI AND F. ROMANI, *Local error estimates in quadrature*, BIT, **31** (1991a), 102–111.
- , G. LOTTI AND F. ROMANI, *Algorithm 691: Improving QUADPACK automatic integration routines*, ACM Trans. Math. Software, **17** (1991b), 218–232.
- L. FEJÉR, *Mechanische Quadraturen mit positiven Cotes'schen Zahlen*, Math. Z., **37** (1933), 287–310.
- W. J. FELTS, *Numerical inversion of the Laplace transform*, IEEE Trans. Automatic Control, **AC-14** (1969), 297–299.
- AND G. E. COOK, *Numerical inversion of the Laplace transform*, IEEE Trans. Automatic Control, **AC-14** (1969), 297–299.
- W. E. FERGUSON, JR., *A simple derivation of Glassman's general N fast Fourier transform*, Comput. Math. Appl., **8** (1982), 401–411.
- S. E. FERRANDO, L. A. KOLASA AND N. KOVACEVIC, *Algorithm 821: A flexible implemen-*

- tation of matching pursuit for Gabor functions on the interval*, ACM Trans. Math. Software, **28** (2002), 337–353.
- S. FILIPPI, *Angenäherte Tschebyscheff-Approximation einer Stammfunktion — eine Modifikation des Verfahrens von Clenshaw und Curtis*, Numer. Math., **6** (1964/29), 320–328.
- L. N. G. FILON, *On a quadrature formula for trigonometric integrals*, Proc. Royal Soc. Edinburgh, **49** (1928/29), 38–47.
- L. FLATTO AND S. HABER, *A quadrature formula of degree three*, J. Approx. Theory, **9** (1971), 44–52.
- A. FLETCHER, J. C. P. MILLER, L. ROSENHEAD AND L. J. COMRIE, *An Index of Mathematical Tables*, 2nd. ed., Addison-Wesley, Reading, MA, 1962.
- E. A. FLINN, *A modification of Filon's method for numerical integration*, J. ACM, **7** (1960), 181–184.
- W. F. FORD AND A. SIDI, *An algorithm for a generalization of the Richardson extrapolation process*, SIAM J. Numer. Anal., **24** (1987), 1212–1232.
- K.-J. FÖRSTER, *On quadrature formulae near Gaussian quadrature*, in Numerical Integration — Recent Developments, Software and Applications (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 45–54.
- E. FOUFOULA-GEORGION AND P. KUMAR (eds.), *Wavelets in Geophysics, Wavelet Analysis and Its Applications*, Vol. 4, Academic Press, San Diego, 1994.
- L. FOX AND I. B. PARKER, *Chebyshev Polynomials in Numerical Analysis*, Oxford Univ. Press, Oxford, 1957.
- P. FRANKLIN, *A set of continuous orthogonal functions*, Math. Ann., **100** (1928), 522–529.
- W. FRASER AND M. W. WILSON, *Remarks on the Clenshaw-Curtis quadrature scheme*, SIAM Rev., **8** (1966), 322–327.
- G. FREUD, *Orthogonale Polynome*, Birkhäuser Verlag, Basel, 1969.
- D. GABOR, *Theory of communications*, J. IEEE, **93** (1946), 429–457.
- B. S. GARBOW, J. M. BOYLE, J. J. DONGARRA AND C. B. MOLER, *Matrix Eigensystem Routines — EISPACK Guide Extension*, Lecture Notes in Computer Science #51, Springer-Verlag, Berlin, 1977.
- , G. GIUNTA, J. N. LYNESS AND A. MURLI, *Software for an implementation of Weeks' method for the numerical inversion of the Laplace transform problem*, ACM Trans. Math. Software, **14** (1988a), 163–170.
- , G. GIUNTA, J. N. LYNESS AND A. MURLI, *Algorithm 662, A Fortran software package for the numerical inversion of the Laplace transform based on Weeks' method*, ACM Trans. Math. Software, **14** (1988b), 171–176.
- AND J. N. LYNESS, *Remark on "Algorithm 662: A Fortran software package for the numerical inversion of the Laplace transform based on Weeks' method"*, ACM Trans. Math. Software, **16** (1990), 405.
- S. GARRIBBA, L. QUARTAPELLE AND G. REINA, *Algorithm 36. SNIFF: Efficient self-tuning algorithm for numerical integration*, Computing, **20** (1978), 363–375.
- J. GARLOFF, W. SOLAK AND Z. SZYDELKO, *New integration formulas which use nodes outside the integration interval*, J. Franklin Inst., **321** (1986), 115–126.
- L. GATTESCHI, *On some orthogonal polynomial integrals*, Math. Comp., **35** (1980), 1291–1298.
- C. F. GAUSS, *Werke*, vol. . 3., 1866, pp. 163–196.
- W. GAUTSCHI, *Construction of Gauss-Christoffel quadrature formulas*, Math. Comp., **22** (1968a), 251–270.
- , *Algorithm 331: Gaussian quadrature Formulas [D1]*, Comm. ACM **11** (1968b), 432–436.
- , *On the condition of a matrix arising in the numerical inversion of the Laplace transform*, Math. Comp., **23** (1969), 109–118.
- , *On the construction of Gaussian rules from modified moments*, Math. Comp., **24** (1970), 245–260.

- , *Quadrature formulae on half-infinite intervals*, BIT, **31** (1991a), 438–446.
- , *On the remainder term for analytic functions of Gauss-Lobatto and Gauss-Radau quadratures*, Rocky Mountain J., **21** (1991b), 209–226; correction, Rocky Mountain J., **21** (1991), 1143.
- , *On the computation of generalized Fermi-Dirac and Bose-Einstein integrals*, Comput. Phys. Comm., **74** (1993), 233–238.
- , *Gauss-type quadrature rules for rational functions*, in Numerical Integration IV (H. Brass and G. Hämmerlin, eds.), Birkhäuser, Basel, 1993a, pp. 110–130.
- , *On the computation of generalized Fermi-Dirac and Bose-Einstein integrals*, Comput. Phys. Communi., **74** (1993b), 233–238.
- , *Algorithm 726: ORTHPOL— A package of routines for generating orthogonal polynomials and Gauss-type quadrature rules*, ACM Trans. Math. Software, **20** (1994), 21–62.
- , *Remark on Algorithm 726: ORTHPOL — A package of routines for generating orthogonal polynomials and Gauss-type quadrature rules*, ACM Trans. Math. Software, **24** (1998), 355–358.
- , *Algorithm 793: GQRAT — Gauss quadrature for rational functions*, ACM Trans. Math. Software, **25** (1999), 213–239.
- AND S. LI, *The remainder term for analytic functions of Gauss-Radau and Gauss-Lobatto quadrature rules with multiple end points*, J. Comp. Anal. Math., **33** (1990), 315–329.
- AND R. S. VARGA, *Error bounds for Gaussian quadrature of analytic functions*, SIAM J. Numer. Math., **20** (1983), 1170–1186.
- AND J. WIMP, *Computing the Hilbert transform for a Jacobi weight function*, BIT, **27** (1987), 203–215.
- W. M. GENTLEMAN, *Implementing Clenshaw-Curtis quadrature, I. Methodology and experience*, Comm. ACM, **15** (1972a), 337–342; 343–346.
- , *Implementing Clenshaw-Curtis quadrature, II. Computing the cosine transformation*, Comm. ACM, **15** (1972b), 343–346.
- , *Algorithm 424: Clenshaw-Curtis quadrature*, Comm. ACM, **15** (1972c), 353–355.
- A. GENZ AND A. A. MALIK, *An imbedded family of fully symmetric numerical integration rules*, SIAM J. Numer. Anal., **20** (1983), 580–588.
- C. F. GERALD AND P. O. WHEATLEY, *Applied Numerical Analysis*, 5th ed., Addison-Wesley, Reading, MA, 1970.
- A. GERASOULIS, *Nyström's iterative variant methods for the solution of Cauchy singular integral equations*, SIAM J. Numer. Anal., **26** (1989), 430.
- AND R. P. SRIVASTAV, *On the solvability of singular integral equations via Gauss-Jacobi quadrature*, BIT, **21** (1982), 377–380.
- , *Piecewise-polynomial quadratures for Cauchy singular integrals*, SIAM J. Numer. Anal., **23** (1986), 891–902.
- IA. L. GERONIMUS, *On Gauss' and Chebychev's quadrature formulas*, Doklady Akad. Nauk SSSR, **51** (1946), 655–658. (Russian)
- , *Theory of Orthogonal Polynomials*, Gostekhizdat, Moscow, 1950.
- A. GHIZZETTI, *Procedure for constructing quadrature formulae on infinite intervals*, Numer. Math., **12** (1968), 111–119.
- AND A. OSSICINI, *Quadrature Formulae*, Birkhäuser, Basel, 1970.
- P. E. GILL AND G. F. MILLER, *An algorithm for the integration of unequally spaced data*, Comput. J., **15** (1972), 80–83.
- G. GIUNTA AND A. MURLI, *Algorithm 649: A package for computing trigonometric Fourier coefficients based on Lyness's algorithm*, ACM Trans. Math. Software, **13** (1987), 97–107.
- , G. LACCETTI AND M. R. RIZZARDI, *More on Weeks method for the numerical inversion of the Laplace transform*, Numer. Math., **54** (1988), 193–200.

- , G. GIUNTA, J. N. LYNESS, AND A. MURLI, *Algorithm 662, A FORTRAN software package for the numerical inversion of the Laplace transform based on Weeks' method*, ACM Trans. Math. Software, **14** (1988b), 171–176.
- I. S. GLADSHTEYN AND I. M. RYZIK, *Tables of Integrals, Series, and Products*, Academic Press, New York, 1965.
- I. GLADWELL, *Vectorization of one-dimensional quadrature codes*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 231–238.
- M. A. GOLBERG AND C. S. CHEN, *Discrete Projection Methods for Integral Equations*, CMP, Southampton and Boston, 1997.
- M. A. GOLDBERG, *Initial value methods in the theory of Fredholm integral equations*, J. Optim. and Appls., **9** (1972), 112–119.
- , *Convergence of an initial value method for solving Fredholm integral equations*, J. Optim. and Appls., **12** (1973), 334–356.
- , *The conversion of Fredholm integral equations to equivalent Cauchy problems*, Appl. Math. and Comput., **2** (1976), 1–18.
- , *The conversion of Fredholm integral equations to equivalent Cauchy problems — Computation of resolvents*, Appl. Math. and Comput., **3** (1977).
- , *Boundary and initial-value methods for solving Fredholm equations with semidegenerate kernels*, J. Optim. Theory and Appls., **24** (1978).
- (ed.), *Solution Methods for Integral Equations*, Plenum Press, New York, 1979.
- , *A method of adjoints for solving some ill-posed equations of the first kind*, J. Appl. Math. and Comput., **5** (1979), 123–130.
- G. H. GOLUB AND J. H. WALSH, *Calculation of Gauss quadrature rules*, Math. Comput., **23** (1969), 221–230.
- E. A. GONZÁLES-VELASCO, *Fourier Analysis and Boundary Value Problems*, Academic Press, San Diego, CA, 1995.
- R. F. GOODRICH AND F. STENGER, *Movable singularities and quadrature*, Math. Comp., **24** (1970), 283–300.
- E. T. GOODWIN, *The evaluation of integrals of the form $\int_{-\infty}^{\infty} f(x)e^{-x^2} dx$* , Proc. Cambr. Philos. Soc., **45** (1949), 241–245.
- E. GOURSAT, *Determination de la resolvante d'une equation Volterra*, Bull. des Scs. et Math. **57** (1933), 144–150.
- , *Cours d'Analyse Mathématique, III*, 5th ed., Gauthier-Villars, Paris, 1934; Dover, New York, 1964.
- A. GRAPS, *An introduction to wavelets*, IEEE Comput. Sc. Engg., **2** (1995).
- H. L. GRAY AND S. WANG, *A new method for approximating improper integrals*, SIAM J. Numer. Anal., **29** (1992), 271–283.
- P. B. GRIDADO, *The transient temperature field in a composite semi-space resulting from an incident heat flux*, Quart. Appl. Math., **31** (1974), 379–393.
- C. W. GROETSCH, *The Theory of Tikhonov Regularization for Fredholm Integral Equations of the First Kind*, Pitman Advanced Publishing Program, Boston, 1984.
- A. GROSSMANN AND J. MORLET, *Decomposition of Hardy functions into square integrable wavelets of constant shape*, SIAM J. Math., **15** (1984), 723–736.
- R. B. GUENTHER AND E. L. ROETMANN, *Newton-Cotes formulas in n dimensions*, Num. Math., **14** (1970), 330–345.
- M. GUIGGIANI, *The evaluation of Cauchy principal value integrals in the boundary element method — A Review*, Math. Comput. Modelling, **15** (1991), 175–184.
- S.-A. GUASTAFSON, *Rapid computation of weights of interpolatory quadrature rules*, CACM, **14** (1971), 807.
- A. HAAR, *Zur Theorie der orthogonalen Funktionensystems*, Math. Ann., **69** (1910), 331–371.
- S. HABER, *Indefinite integration formulas based on the sinc expansion*, in Numerical In-

- tegration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 105–106.
- W. HACKBUSCH, *Multigrid Methods and Applications*, Springer-Verlag, Berlin, 1985.
- , *Integral Equations*, Birkhäuser, Boston, 1995.
- J. HADAMARD, *Lectures on Cauchy's Problem in Linear Partial Differential Equations*, Yale Univ. Press, New Haven, 1923.
- D. F. HAINES, *Numerical Inversion of Laplace Transforms and Applications*, M.S. Thesis, University of New Orleans, New Orleans, LA, May 1982.
- O. T. HANNA AND L. F. BROWN, *A new method for the numerical solution of Fredholm integral equations of the first kind*, Chemical Engg. Soc., **46** (1991), 2749–2753.
- P. C. HAMMER, O. J. MARLOWE AND A. H. STROUD, *Numerical integration over simplexes and cones*, Math. Tables Aids Comput., **10** (1956), 130–137.
- AND A. W. WYMORE, *Numerical evaluation of multiple integrals I*, Math. Tables Aids Comput., **11** (1957), 59–67.
- AND H. H. WICKE, *Quadrature formulas involving derivatives of the integrand*, Math. Comp., **14** (1960), 3–7.
- P. C. HANSEN, *Numerical tools for analysis and solution of Fredholm integral equations of the first kind*, Inverse Problems, **8** (1992), 849–887.
- C. G. HARRIS AND W. A. B. EVANS, *Extension of numerical quadrature formulae to cater for end-point singular behaviour over finite intervals*, Int. J. Comp. Math., **6** (1977), 219–227.
- T. HASEGAWA AND T. TORII, *An automatic quadrature for Cauchy principal value integrals*, Math. Comp., **56** (1991), 741–754.
- AND T. TORII, *Hilbert and Hadamard transforms by generalized Chebyshev expansion*, J. Comput. Appl. Math., **51** (1994), 71–83.
- A. HAUSNER, *NL9 — An adaptive routine for numerical quadrature*, Proc. 1977 Army Numer. Anal. Comput. Conf., (1977), 367–410.
- AND J. D. HUTCHISON, *FOGIE: An adaptive code for numerical integrals using Gaussian quadrature*, Proc. 1975 Army Numer. Anal. Comput. Conf., (1975), 139–177.
- P. HENRICI, *Elements of Numerical Analysis*, Wiley, New York, 1964.
- E. HERNÁNDEZ AND G. WEISS, *A First Course on Wavelets*, CRC Press, Boca Raton, FL, 1996.
- J. H. HETHERINGTON, *An error bound for quadrature*, Math. Comput., **26** (1972), 695–698.
- J. HEINHOLD, *Einige mittels Laplace-Transformation lösbare Integralgleichungen, I*, Math. Z., **52** (1950), 779–790.
- P. HENRICI, *Elements of Numerical Analysis*, Wiley, New York, 1964.
- R. B. HETNARSKI, *On inverting the Laplace transforms connected with the error function*, Zastowania Matem., **7** (1964), 399–405.
- , *An algorithm for generating some inverse Laplace transforms of exponential form*, ZAMP, **26** (1975), 249–254.
- F. B. HILDEBRAND, *Introduction to Numerical Analysis*, McGraw-Hill, New York, 1956; 2nd ed., 1974, pp. 389.
- H. HOCHSTADT, *Integral Equations*, John Wiley, New York, 1973.
- G. HONIG AND U. HIRDES, *A method for the numerical inversion of Laplace transforms*, J. Comput. Appl. Math., **10** (1984), 113–132.
- T. H. HOPP, *A routine for numerical evaluation of integrals with oscillatory integrands*, Proc. 1977 Army Numer. Anal. Comput. Conf., (1979), 187–221.
- R. W. HORNBECK, *Numerical Methods*, Quantum Publishers, New York, 1975.
- C. B. HUELSMAN, III, *Quadrature formulae over fully symmetric planar regions*, SIAM J. Numer. Anal., **10** (1973), 539–552.
- J. HUMLECEK, *An efficient method for evaluation of complex probability integral: the Voigt function and its derivatives*, J. Quart. Spectros. Radiol. Transfer, **121** (1979), 309–313.
- D. B. HUNTER, *The evaluation of integrals of periodic analytic functions*, BIT, **11** (1971),

- 175–180.
- , *Some error expansions for Gaussian quadrature*, BIT, **35** (1995), 64–82.
- , *The numerical evaluation of definite integrals affected by singularities near the interval of integration*, in *Numerical Integration — Recent Developments, Software and Applications* (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 111–120.
- AND G. E. OKECHA, *A modified Gaussian quadrature rule for integrals involving poles of any order*, BIT, **26** (1986), 233–240.
- AND G. NIKOLOV, *Gauss-Lobatto quadrature formulas associated with symmetric weight functions*, Math. Comp., **69** (1999), 269–282.
- B. HÜPPER AND E. POLLAK, *Numerical inversion of the Laplace transform*, J. Chem. Phys., **110** (1999), 11176–11186.
- H. HURWITZ AND P. F. ZWEIFEL, *Numerical quadrature of Fourier transform integrals*, MTAC, **10** (1956), 140–149.
- , R. A. PFEIFER AND P. F. ZWEIFEL, *Numerical quadrature of Fourier transform integrals, II*, MTAC, **13** (1959), 89–90.
- C. HWANG AND M.-J. LU, *Improved FFT-based numerical inversion of Laplace transforms via fast Hartley transform algorithm*, Computers Math. Applic., **22** (1991), 13–24.
- IBM, *System/360 Scientific Subroutine Package, Version III. Programmer's Manual H20-0205-3*, 1968.
- J. P. IMHOF, *On the method for numerical integration of Clenshaw and Curtis*, Numer. Math., **5** (1963), 138–141.
- H. INOUE, M. KAMIBAYASHI, K. KISHIMOTO, T. SHUBIYA AND T. KOIZUMI, *Numerical Laplace transformation and inversion using fast Fourier transform*, JSME Intern. J., Ser. I, **35** (1992), 319–324.
- N. I. IOAKIMIDIS, *On the uniform convergence of Gaussian quadrature rules for Cauchy principal value integrals and their derivatives*, Math. Comp., **44** (1985), 191–198.
- , *Mangler-type principal value integrals in hypersingular integral equations for crack problems in plane elasticity*, Engg. Frac. Mech., **31** (1988), 895–898.
- , *Application of computer algebra software to the derivation of numerical integration rules for singular and hypersingular integrals*, in *Numerical Integration — Recent Developments, Software and Applications* (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 121–131.
- AND P. S. THEOCARIS, *On the numerical evaluation of Cauchy principal value integrals*, Rev. Roumaine Sci. Tech. Sér. Méc. Appl., **22** (1977), 803–818.
- M. IRI, S. MORIGUTI, AND Y. TAKASAWA, *On a certain quadrature formula*, Kokyuroku of the research Inst. for Math. Scs., Kyoto Univ., **91** (1970), 82–118. (Japanese)
- M. A. JAWSON, *Integral equation methods in potential theory, I*, Proc. Royal Soc., **A 275** (1963), 23–32 (for part II, see [G. T. Symm](#)).
- E. ISAACSON AND H. B. KELLER, *Analysis of Numerical Methods*, Wiley, New York, 1966.
- E. JEN AND R. P. SRIVASTAV, *Solving singular integral equations using Gaussian quadrature and overdetermined systems*, Comp. & Maths. with Appls., **9** (1983), 625–632.
- A. J. JERRI, *Integral and Discrete Transforms with Applications and Error Analysis, Vol. 162, Monograph Textbooks Pure Appl. Math.*, Maecel Dekker, New York, 1992.
- B. JONES, *A note on the T transformation*, Nonlinear Analysis: Theory, Methods and Applications, **6** (1982), 303–305.
- L. W. JOHNSON AND R. D. RIESS, *Minimal quadratures of low order continuity*, Math. Comput., **25** (1971), 832–835.
- AND R. D. RIESS, *Numerical Analysis*, Addison-Wesley, Reading, MA, 1977.
- , R. D. RIESS, AND J. T. ARNOLD, *Introduction to Linear Algebra*, 2nd ed., Addison-Wesley, Reading, MA, 1993.
- W. W. JOHNSON, *On Cotesian numbers: their history, computation and values*, Quart. J. Pure Appl. Math., **46** (1915), 52–65.
- P. M. JORDAN, P. PURI, AND G. BOROS, *A new class of Laplace inverses and their appli-*

- cations, *Applied Math. Letters*, **13** (2000), 97–104.
- , M. R. MEYER, AND A. PURI, *Causal implications of viscous damping in compressible fluid flows*, *Physical Review, E*, **62** (2000), 7981–7926.
- H. KABIR, E. MADENCI, AND A. ORTEGA, *Numerical solution of integral equations with logarithmic-, Cauchy- and Hadamard-type singularities*, *Intl. J. Numer. Methods in Engg.*, **41** (1998), 617–638.
- H. KADNER, *Die numerische Behandlung von Integralgleichungen nach der Kollokationsmethode*, *Numer. Math.* **10** (1967), 241–261.
- D. K. KAHANER, *Comaprison of numerical quadrature formulae*, in *Mathematical Software* (J. R. Rice, eds.), *ACM Monograph Series*, Academic Press, London, 1971, pp. 229–259.
- , *Numerical quadrature by the ε -algorithm*, *Math. Comp.*, **26** (1972), 689–693.
- , M. KLERER AND F. GROSSMAN, *Error rates in tables of indefinite integrals*, *Indust. Math.*, **18** (1968), 31–62.
- AND G. MONEGATO, *Nonexistence of extended Gauss-Laguerre and Gauss-Hermite quadrature rules with positive weights*, *ZAMP*, **29** (1978), 983–986.
- , *Development of useful quadrature software with particular emphasis on microcomputers*, in *Numerical Integration — Recent Developments, Software and Applications* (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 343–369.
- G. KAISER, *A Friendly Guide to Wavelets*, Birkhauser, Boston, 1994, pp. 44–45.
- J. KAJIWARA AND M. TSUJI, *Inverse formula for Laplace transform*, 5th Intern. Colloq. on Diff. Eqs (D. Bainov and V. Covachev, eds.), VSP, 1995, pp. 163–173.
- AND M. TSUJI, *Program for the numerical analysis of inverse formula for Laplace transform*, Second Korean-Japanese Colloq. on Finite or Infinite Complex Analysis (1995), 93–107.
- A. I. KALANDIYA, *Mathematical Methods for Two-Dimensional Elasticity*, Mir Publs., Moscow, 1973.
- D. W. KAMMLER, *A First Course in Fourier Analysis*, Prentice Hall, Upper Saddle River, NJ, 2000.
- H. KANEKO, *A projection method for solving Fredholm integral equations of the second kind*, *Trans. Appl. Numer. Math.*, **5** (1989), 333.
- AND Y. XU, *Numerical solutions for weakly singular Fredholm integral equations of the second kind*, *Trans. Appl. Numer. Math.*, **7** (1991), 167–177.
- AND R. NOREN, *An application of approximation theory to numerical solutions for Fredholm integral equations of the second kind*, *Numer. Functional Anal. Optim.*, **5** (1992), 517.
- , R. D. NOREN, AND Y. XU, *Numerical solutions for weakly singular Hammerstein equations and their superconvergence*, *J. Integral Eqns. Appls.*, **4** (1992), 391.
- R. P. KANWAL, *Linear Integral Equations*, Academic Press, New York, 1971.
- , *Linear Integral Equations*, Birkhäuser, Boston, 1997.
- L. V. KANTOROVICH AND V. I. KRYLOV, *Approximate Methods for Higher Analysis*, Interscience, New York, 1958.
- AND G. P. AKILOV, *Functional Analysis in Normed Spaces*, Pergamon Press, Oxford, 1964.
- J. KAUSKY AND S. ELHAY, *Calculation of the weights of interpolatory quadratures*, *Numer. Math.*, **40** (1982), 407–422.
- A. C. KAYA AND F. ERDOGAN, *On the solution of integral equations with strongly singular kernels*, *Quarterly Appl. Math.*, **45** (1987), 105–122.
- P. KEAST AND J. N. LYNES, *On the structure of fully symmetric multidimensional quadrature rules*, *SIAM J. Numer. Anal.*, **16** (1979), 11–29.
- AND G. FAIRWEATHER (eds.), *Numerical Integration — Recent Developments, Software and Applications*, D. Reidel, Dordrecht, the Netherlands, 1987.
- C. T. KELLEY, *Solution of the Chandrasekhar H-equation by Newton's method*, *J. Math.*

- Phys., **21** (1982), 1625–1628.
- , *A fast multilevel algorithm for integral equations*, SIAM J. Numer. Anal., **32** (1995), 501–513.
- J. T. KING, *Introduction to Numerical Computation*, McGraw-Hill, New York, 1984.
- K. KNOPP, *Theory and Applications of Infinite Series*, Blackie & Son, Ltd., London, 1928.
- J. KONDO, *Integral Equations*, Kodansha, Tokyo, and Clarendon Press, Oxford, 1991.
- Z. KOPAL, *Numerical Analysis*, 2nd ed., Wiley, New York, 1961.
- G. KOWALEWSKI, *Interpolation und Genährte Quadratur*, Teubner, Leipzig, 1932.
- W. KRÄMER AND S. WENDER, *Two adaptive Gauss-Legendre type algorithms for the verified computation of definite integrals*, Reliable Computing, **2** (1996), 241–254.
- H. L. KRALL AND O. FRINK, *A new class of orthogonal polynomials*, Trans. Amer. Math. Soc., **65** (1949), 100–145.
- S. KRENK, *On quadrature formulas for singular integral equations of the first and second kind*, Quart. Appl. Math., (Oct. 1975), 225–232.
- , *Quadrature formulas of closed type for the solution of singular integral equations*, J. Inst. Math. Appl., **22** (1978), 99–107.
- R. KRESS, *Linear Integral Equations*, Springer-Verlag, Berlin, 1989.
- , I. SLOAN, AND F. STENGER, *A sinc quadrature method for the double-layer integral equation in planar domains with corners*, J. Integral Eqns. Appl., **10** (1998), 291–317.
- A. S. KRONROD, *Nodes and Weights of Quadrature Formulas*, Consultants Bureau, New York, 1965.
- F. T. KROGH AND W. VAN SNYDER, *Algorithm 699: A new representation of Patterson's quadrature formulae*, ACM Trans. Math. Software, **17** (1991), 457–461.
- V. I. KRYLOV, *Approximate Calculation of Integrals* (Russian); English transl. by A. Stroud, Macmillan, New York, 1962.
- , V. V. LUGIN AND L. A. YANAVICH, *Tables of Numerical Integration for $\int_0^1 x^\beta (1-x)^\alpha f(x) dx$* , Akademiya Nauk Belorusskoi S. S. R., Minsk, 1963 (Russian).
- AND L. G. KRUGLIKOVA, *Handbook on Numerical Harmonic Analysis*, Nauka i Tekhnika, Minsk, 1968 (Russian).
- AND N. S. SKOBLYA, *On the numerical inversion of the Laplace transform*, Inzh.-Fiz. Zh., **4** (1961), 85–101. (Russian)
- AND A. A. PAL'TSEV, *Tables for Numerical Integration of Functions with Logarithmic and Power Singularities*, Israel Program for Scientific Translation, Jerusalem, 1974.
- AND N. S. SKOBLYA, *A Handbook of Numerical Inversion of Laplace Transforms*, Mir Publishers, Moscow, 1977.
- E. KREYSZIG, *Introductory Functional Analysis with Applications*, John Wiley, New York, 1978.
- P. K. KULSHRESTHA AND P. PURI, *An exact solution of hydromagnetic boundary layer in a rotating medium*, Proc. 11th Midwestern Mech. Conf., Developments in Mech., **5** (1969), 265–271.
- G. F. KUNCIR, *Algorithm 103. Simpson's rule integrator*, Comm. ACM, **5** (1962), 347.
- S. S. KUO, *Computer Applications of Numerical Methods*, Addison-Wesley, Reading, MA, 1972.
- R. D. KURTZ, T. N. FARRIS, AND C. T. SUN, *The numerical solution of Cauchy singular integral equations with application of fracture*, Intl. J. Fracture, **66** (1994), 139.
- H. R. KUTT, *Quadrature Formulas for Finite-Part Integrals*, Special Report WISK, **178**, National Research Institute for Mathematical Sciences, Pretoria, South Africa (1975).
- , *On the numerical evaluation of finite-part integrals involving an algebraic singularity*, CSIR Special Report WISK, Pretoria, **179** (1976).
- , *On the numerical evaluation of principal value integrals by finite-part integration*, Numer. Math., **24** (1975), 205–210.
- , *Gaussian quadrature formulae for improper integrals involving a logarithmic sin-*

- gularity, CSIR Special Report WISK, Pretoria, **1232** (1976).
- P. K. KYTHE, *An Introduction to Boundary Element Methods*, CRC Press, Boca Raton, FL, 1995.
- , *Fundamental Solutions for Differential Operators and Applications*, Birkhäuser, Boston, 1996.
- , *Computational Conformal Mapping*, Birkhäuser, Boston, 1998.
- P. PURI and M. R. SCHÄFERKOTTER, *Partial Differential Equations and Mathematica*, CRC Press, Boca Raton, FL, 1997.
- AND P. PURI, *Computational Methods for Linear Integral Equations*, Birkhäuser, Boston, 2002.
- P. PURI and M. R. SCHÄFERKOTTER, *Partial Differential Equations and Boundary Value Problems with Mathematica*, CRC Press, Boca Raton, FL, 2002.
- AND D. WEI, *An Introduction to Linear and Nonlinear Finite Element Analysis*, Birkhäuser, Boston, 2004.
- G. LACCETTI, *The incidental parameters of a numerical method for inverting a Laplace transform function*, *Ricerche di Matem.*, **41** (1992), 163–184.
- C. LANCZOS, *Applied Analysis*, Prentice-Hall, Englewood Cliffs, NJ, 1956.
- P. J. LAURENT, *Formules de quadrature approchée sur domines rectangulaires convergentes pour toute fonction intégrable Riemann*, *C. R. Acad. Sci. Paris*, **258** (1964), 798–801.
- D. P. LAURIE, *Sharpoer error estimates in adaptive quadrature*, *BIT*, **23** (1983), 256–261.
- , *Null rules and orthogonal expansions*, in *Approximation and Computation: A Festschrift in Honor of Walter Gautschi* (R. V. M. Zahar, eds.), Vol. 119 of *Internatal Ser. Numer. Math.*, Birkhäuser, Boston, 1994, pp. 350–370.
- AND L. ROLFES, *Algorithm 015. Computation of Gaussian quadrature rules from modified moments*, *J. Comput. Appl. Math.*, **5** (1979), 235–242.
- AND A. VENTER, *Automatic Quadrature of Functions of the Form $|f(x)|$* , Technical Note T/15, Potchefstroom University, 1993.
- M. M. LAVRENTIEV, *Some Improperly Posed Problems of Mathematical Physics*, Springer-Verlag, New York, 1967.
- D. LAZARD AND R. RIOBOO, *Integration of rational functions — Rational computation of the logarithmic part*, *J. Symbolic Comput.*, **9** (1990), 113–115.
- F. LETHER, *Modified quadrature formulas for functions with nearby poles*, *J. Comp. Appl. Math.*, **3** (1977), 3–9.
- , *Analytical expansions for the numerical approximation of the Fermi-Dirac integrals $F_j(x)$ of order $j = -1/2$ and $j = 1/2$* , *J. Sci. Comput.*, **15** (2000), 479–497.
- , *Variable precision algorithm for the numerical computation of the Fermi-Dirac function $F_j(x)$ of order $j = -3/2$* , *J. Sci. Comput.*, **16** (2001), 69–79.
- D. LEVIN, *Development of non-linear transformations for improving convergence of sequences*, *Int. J. Comp. Math.*, **3** (1973), 371–388.
- , *Numerical inversion of Laplace transforms by accelerating the convergence of Bromwich's integrals*, *J. Comp. Appl. Math.*, **1** (1975), 247–257.
- , *Procedures for computing one and two dimensional integrals of functions with rapid irregular oscillations*, *Math. Comp.*, **38** (1982), 531–538.
- AND A. SIDI, *Two new classes of non-linear transformations for accelerating the convergence of infinite integrals and series*, *Appl. Math. Comp.*, **9** (1981), 175–215.
- N. LEVINSON, *Simplified treatment of integrals of Cauchy type, the Hilbert problem and singular integral equations*, *SIAM Rev.*, **7** (1965), 474–502.
- S. LEWANOWICZ, *Construction of a recurrence relation for modified moments*, *J. Comp. Appl. Math.*, **5** (1979), 193–206.
- , *Recurrence relations for modified moments*, *Rev. T'ec. Ing., Univ. Zulia*, **8** (1985), 49–60.
- M. J. LIGHTHILL, *Fourier Analysis and Generalized Functions*, Cambridge Univ. Press, Cambridge, 1959.

- P. LINZ, *Numerical methods for Volterra integral equations of the first kind*, Comput. J., **12** (1969), 393–397.
- , *Product integration methods for Volterra integral equations of the first kind*, BIT, **11** (1971), 413–421.
- , *Algorithm 427. Fourier cosine integral*, Comm. ACM, **15** (1972), 358–360.
- , *An analysis of a method for solving singular integral equations*, BIT, **17** (1977), 329–337.
- , *Analytical and numerical methods for Volterra equations*, SIAM Stud. Appl. Math., 1985.
- , *Bounds and estimates for condition numbers of integral equations*, SIAM J. Numer. Anal., **28** (1991), 227.
- R. LIPOW AND F. STENGER, *How slowly can quadrature formulae converge?*, Math. Comput., **26** (1972), 917–922.
- J. E. LITTLEWOOD AND R. E. A. C. PALEY, *Theorems on Fourier series and power series*, I, J. London Math. Soc., **6** (1931), 230–233.
- AND R. E. A. C. PALEY, *Theorems on Fourier series and power series*, II, Proc. London Math. Soc., **42** (1936), 52–89.
- F. LOCHER AND K. ZELLER, *Approximationsgüte und numerische Integration*, Math. Zeit., **104** (1968), 249–251.
- I. M. LONGMAN, *A method for the numerical evaluation of finite integrals of oscillatory functions*, Math. Comp., **14** (1960), 53–59.
- W. V. LOVITT, *Linear Integral Equations*, Dover, New York, 1950.
- D. W. LOZIER, *Numerical solution of linear difference equations*, Report NBSIR 80-1976 (1980), National Bureau of Standards, Washington, D.C.
- L. C. MAXIMON AND W. L. SADOWSKI, *A bit comparison program for algorithm testing*, Comput. J., **16** (1973), 111–117.
- J. LU, *A class of quadrature formulas of Chebyshev type for singular integrals*, J. Math. Anal. Appl. (2), **100** (1984), 416–435.
- D. S. LUBINSKY AND P. RABINOWITZ, *Rates of convergence of Gaussian quadrature for singular integrands*, Math. Comp., **43** (1984), 219–242.
- AND A. SIDI, *Convergence of product integration rules for functions with interior and endpoint singularities*, Math. Comp., **46** (1986), 229–245.
- Y. L. LUKE, *Integrals of Bessel Functions*, McGraw-Hill, New York, 1962.
- , *Approximations of elliptic integrals*, Math. Comp., **22** (1968), 627–634.
- , *The Special Functions and Their Approximations*, Vol. 2, Academic Press, New York, 1969, pp. 255–269.
- J. LUND, *Sinc function quadrature rules for the Fourier integral*, Math. Comp., **41** (1983), 103–113.
- AND K. L. BOWERS, *Sinc Methods for Quadrature and Differential Equations*, SIAM, Philadelphia, 1992.
- J. N. LYNESS, *The effect of inadequate convergence criteria in automatic routines*, Computer J., **12** (1969), 279–281.
- , *Algorithm 379. SQUANK (Simpson quadrature used adaptively — Noise killed)*, Comm. ACM, **13** (1970), 260–263; **15** (1972), 1073.
- , *When not to use an automatic quadrature routine*, SIAM Rev., **25** (1983), 63–87.
- , *Notes on the adaptive Simpson quadrature routine*, J. ACM, **16** (1969), 483–495.
- , *Guidelines for Automatic Quadrature Routines*, in Information Processing 71 (C. V. Freeman et al., eds.), vol. 2, North-Holland, Amsterdam, 1972.
- , *Computational techniques based on Lanczos representation*, Math. Comp., **28** (1974), 81–123.
- , *The calculation of trigonometric Fourier coefficients*, J. Comp. Phys., **54** (1984), 57–73.
- , *Some quadrature rules for finite trigonometric and related integrals*, in Numerical-

- cal Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 17–34.
- , *Finite-part integrals and the Euler-Maclaurin expansion*, in Approximation and Computation: A Festschrift in Honor of Walter Gautschi (R. V. M. Zahar., eds.), Vol. 119 of Internat. Ser. Numer. Math., Birkhäuser, Boston, 1994, pp. 397–407.
- AND E. DE DONCKER, *On quadrature error expansions, I*, J. Comp. Appl. Math., **17** (1987), 131–149.
- AND E. DE DONCKER, *On quadrature error expansions, II — The full corner singularity*, Numer. Math., **64** (1993), 355–370.
- AND G. GIUNTA, *A modification of the Weeks method for the numerical inversion of Laplace transforms*, Math. Comput., **47** (1986), 313–322.
- AND D. JESPERSEN, *Moderate degree symmetric quadrature rules for the triangle*, J. Inst. Math. Appl., **15** (1975), 19–32.
- AND B. W. NINHAM, *Numerical quadrature and asymptotic expansions*, J. Math. Comp., **21** (1967), 162–178.
- A. J. MACLEOD, *Algorithm 779: Fermi-Dirac functions of order $-1/2, 1/2, 3/2, 5/2$* , ACM Trans. Math. Soft., **24** (1998), 1–12.
- M. A. MALCOLM AND R. B. SIMPSON, *Local versus global strategies for adaptive quadrature*, ACM Trans. Math. Software, **1** (1975), 129–146.
- S. MALLET, *Multiresolution approximations and wavelet orthonormal bases for $L^2(\mathbb{R})$* , Trans. Amer. Math. Soc., **315** (1989a), 60–87.
- , *A theory of multiresolution signal decomposition: the wavelet representation*, IEEE Trans. Pattern Anal. Machine Intell., **11** (1989b), 674–693.
- J. T. MARTI, *Introduction to the Theory of Bases*, Springer-Verlag, Berlin, 1969.
- H. MARVAR, *Lapped transforms for efficient transform/subband coding*, IEEE Trans. Acoustics Speech Signal and Processing, **38** (1990), 969–978.
- G. MASTROIANNI AND G. MOGENATO, *Polynomial approximations of functions with end-point singularities and product integration formulas*, Math. Comp., **62** (1994), 725–738.
- AND S. PROSSDORF, *Some nodes matrices appearing in the numerical analysis for singular integral equations*, BIT, **34** (1994), 120.
- AND G. MOGENATO, *Convergence of product integration rules over $(0, \infty)$ for functions with weak singularities at the origin*, Math. Comp., **64** (1995), 237–249.
- N. W. MCLACHLAN, *Complex Variables and Operational Calculus*, 2nd ed., Macmillan, New York, 1953.
- J. MCNAMEE, *Error-bounds for the evaluation of integrals by the Euler-Maclaurin formula and by Gauss-type formulae*, Math. Comp., **18** (1964), 368–381.
- , *A program to integrate a function tabulated at unequal intervals*, Intern. J. Numer. Methods in Engg., **17** (1981), 271–279.
- W. S. MEISEL, *A numerical integration formula useful in Fourier analysis*, Commun. ACM, **11** (1968), 51.
- Y. MEYER, *Wavelets and Operators*, (Translation from ‘Ondelettes et Opérateurs. I: Herman, Paris, 1990), Cambridge Univ. Press, 1992.
- , *Wavelets, Algorithms and Applications*, SIAM, 1993.
- C. A. MICCHELLI AND T. J. RIVLIN, *Numerical integration rules near Gaussian quadrature*, Israel J. Math., **16** (1973), 287–299.
- G. MIEL, *Parallel solution of Fredholm integral equations on the second kind by orthogonal polynomial expansions*, Trans. Appl. Numer. Math., **5** (1989), 345.
- S. G. MIKHLIN, *Integral Equations*, Pergamon Press, Oxford, 1957.
- , *Linear Integral Equations*, Hindustan Publ. Corp., Delhi, 1960.
- , *Linear Equations of Mathematical Physics*, Holt, Reinhart and Winston, New York, 1967.
- , *The Numerical Performance of Variational Methods*, Noordhoff, Gröninge, 1971; from Russian.

- AND K. L. SMOLITSKIY, *Approximate Methods for Solution of Differential and Integral Equations*, American Elsevier Publishing Co. Inc., New York, 1967.
- E. K. MILLER, *A variable interval width quadrature technique based on Romberg's method*, J. Comput. Phys., **5** (1970), 265–279.
- J. C. P. MILLER, *Quadrature in terms of equally spaced function values*, Tech. Summary Rep. 167, Math. Res. Center, Madison, WI, 1960.
- M. MILLER AND W. T. GUY, JR., *Numerical inversion of the Laplace transform by the use of Jacobi polynomials*, SIAM J. Numer. Anal., **3** (1966), 624–635.
- R. K. MILLER, *On ignoring the singularity in numerical quadrature*, Math. Comp., **25** (1971), 521–532.
- M. MISITI, Y. MISITI, G. OPPENHEIM AND J.-M. POGGI, *Wavelet Toolbox*, Version 2, The MathWorks, Natick, Ma, 1997–2000.
- J. L. MOHAMED AND J. E. WALSH, *Numerical Algorithms*, Clarendon Press, Oxford, 1986.
- G. MONEGATO, *A note on extended Gaussian quadrature rules*, Math. Comp., **30** (1976), 812–817.
- , *Stieltjes polynomials and related quadrature rules*, SIAM Rev., **24** (1982), 137–158.
- , *Quadrature formulas for functions with poles near the interval of integration*, Math. Comp., **47** (1986), 301–312.
- , *Quadrature formulas for functions with poles near the interval of integration*, Math. Comp., **47** (1986), 301–312.
- , *On the weights of certain quadratures for the numerical evaluation of Cauchy principal value integrals and their derivatives*, Numer. Math., **50** (1987), 273–281.
- , *On the weights of certain quadratures for the numerical evaluation of Cauchy principal value integrals and their derivatives*, Numer. Math., **50** (1987), 273–281.
- , *The numerical evaluation of a 2-D Cauchy principal value integral arising in boundary integral equation method*, Math. Comp., **62** (1994), 765–777.
- , *Numerical evaluation of hypersingular integrals*, J. Comput. Appl. Math., **50** (1994), 9–31.
- , *The numerical evaluation of a 2-D Cauchy principal value integral arising in boundary integral equation method*, Math. Comp., **62** (1994), 765–777.
- , *Numerical evaluation of hypersingular integrals*, J. Comput. Appl. Math., **50** (1994), 9–31.
- D. M. MONROE, *Algorithm AS 83. Complex discrete fast Fourier transform*, Appl. Statistics, **24** (1975), 153–160.
- , *Algorithm AS 97. Real discrete fast Fourier transform*, Appl. Statistics, **25** (1976), 166–172.
- AND J. L. BRANCH, *Algorithm AS 117. The Chirp discrete fast Fourier transform of general length*, Appl. Statistics, **26** (1977), 351–361.
- B. P. MOORS, *Valeur Approximative d'une Intégrale Définie*, Gauthier-Villars, Paris, 1905.
- C. R. MORROW, *A Study of Some Numerical Quadrature and Cubature Processes*, Ph.D. Thesis, Belfast, 1977.
- G. MÜHLBACH, *Neville-Atkin algorithms for interpolating by functions of Chebyshev-systems in the sense of Newton and in a generalized sense of Hermite*, in *Theory of Approximations with Applications* (A. G. Law and B. N. Sahney, eds.), Academic Press, New York, 1976, pp. 200–212.
- A. MURLI AND V. PATRUNO, *Un metodo per l'inversione numerica della trasformata de Laplace*, Calcolo, **15** (1978).
- AND M. RIZZARDI, *Algorithm 682: Talbot's method for the Laplace inversion problem*, ACM Trans. Math. Software, **16** (1990), 158–168.
- M. J. P. MUSGRAVE AND J. TASI, *Shock waves in diatomic chains. I. Linear analysis*, J. Mech. Phys. Solids, **24** (1976), 19–42.
- N. I. MUSHKHELISHVILI, *Singular Integral Equations*, Dover Publications, New York, 1992.
- G. MYERSON, *On ignoring singularity*, SIAM J. Numer. Anal., **28** (1991), 1803–1807.

- NAG LTD., *NAG Fortran Library Manual — Mark 17*, Numerical Analysis Group, NAG Central Office, Oxford, 1996.
- M. T. NAIR, *A unified approach for regularized approximation methods for Fredholm integral equations of the first kind*, Numer. Functional Anal. Optim., **15** (1994), 381.
- I. P. NATANSON, *Constructive Function Theory, I*, Ungar, New York, 1964.
- NBS HANDBOOK, *Handbook of Mathematical Functions*, National Bureau of Standards, Applied Math. Series, No. 55, U.S. Govt. Printing Office, Washington, DC, 1964.
- P. NEVAI, *Mean convergence of Lagrange interpolation. III*, Trans. Amer. Math. Soc., **282** (1984), 669–698.
- Y. NIEVERGELT, *Wavelets Made Easy*, Birkhäuser, Boston, 1999.
- B. NOBLE, *The Numerical Solution of Integral Equations*, in *The State of the Art in Numerical Analysis* (D. A. H. Jacobs, ed.), Academic Press, New York, 1977.
- N. A. NODA AND T. MATSUO, *Numerical solutions of singular integral equations having Cauchy-type singular kernel by means of expansion method*, Intl. J. of Fracture, **63** (1993), 229.
- H. V. NORDÉN, *Numerical inversion of the Laplace transform*, Acta Acad. Aboensis Matem. et Physica, **22** (1961), 1–30.
- S. E. NOTARIS, *An overview of results on the existence or nonexistence and the error term of Gauss-Kronrod quadrature formulae*, in *Approximation and Computation: A Festschrift in Honor of Walter Gautschi* (R. V. M. Zahar, eds.), Vol. 119 of Internat. Ser. Numer. Math., Birkhäuser, Boston, 1994, pp. 485–496.
- H. H. NUTALL, *Some windows with very good sidelobe behavior*, IEEE Trans. of Acoustics Speech and Signal Processing (ASSP), **29** (1980), 84.
- E. J. NYSTRÖM, *Über die praktische Auflösung von Integralgleichungen mit Anwendungen auf Randwertaufgaben*, Acta Math., **54** (1930), 185–204.
- F. OBERHETTINGER AND L. BADU, *Tables of Laplace Transforms*, Springer-Verlag, Berlin, New York, 1973.
- W. C. OBI, *Error analysis of a Laplace transform inversion procedure*, SIAM J. Numer. Anal., **27** (1990), 457–469.
- H. O'HARA AND F. H. SMITH, *Error estimation in the Clenshaw-Curtis quadrature formulae*, Computer J., **11** (1968), 213–219.
- AND F. J. SMITH, *The evaluation of definite integrals by interval subdivision*, Computer J., **12** (1969), 179–182.
- M. A. O'NEILL, *Faster Than Fast Fourier*, BYTE, (April 1988), 293–300.
- T. OOURA AND M. MORI, *A double exponential formula for oscillatory functions over the half infinite interval*, J. Comput. Appl. Math., **38** (1991), 353–360.
- D. F. PAGET, *Generalized Product Integration*, Ph. D. Thesis, University of Tasmania, Hobart, 1976.
- , *The numerical evaluation of Hadamard finite-part integrals*, Numer. Math., **36** (1981), 447–453.
- A. PALAMARA-ORSI, *Two algorithms for the construction of product formulas*, Computing, **49** (1993), 367–372.
- R. E. A. C. PALEY, *A remarkable system of orthogonal functions*, Proc. London Math. Soc., **34** (1932), 241–279.
- AND A. ZYGMUND, *On some series of functions*, Proc. Cambridge Phil. Soc., **34** (1930), 337–357, 458–474, (1932), 190–205.
- G. PANTIS, *The evaluation of integrals with oscillatory integrands*, J. Comp. Phys., **17** (1975), 229–233.
- Y. C. PAO, *Engineering Analysis*, CRC Press, Boca Raton, FL, 1999.
- A. PAPOULIS, *A new method of inversion of the Laplace transform*, Quart. Appl. Math., **14** (1956), 405–414.
- , *Signal Analysis*, 4th ed., McGraw-Hill, New York, 1988.
- T. N. L. PATTERSON, *The optimal addition of points to quadrature formulae*, Math. Comp.,

- 22** (1968), 847–856.
- , *On some Gauss and Lobatto based integration formulae*, Math. Comp., **22** (1968), 877–881.
- , *Integration formulas using derivatives*, Math. Comp., **23** (1969), 411–412.
- , *Algorithm 468. Algorithm for automatic numerical integration over a finite interval*, Comm ACM, **16** (1973), 694–699.
- , *On high precision methods for the evaluation of Fourier integrals with finite and infinite limits*, Numer. Math., **27** (1976), 41–52.
- , *On the construction of a practical Ermakov-Zolotukhin multiple integration*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 269–290.
- , *An algorithm for generating interpolatory quadrature rules of the highest degree of precision with preassigned nodes for general weight function*, ACM Trans. Math. Software, **15** (1989a), 123–136.
- , *Algorithm 672: Generation of interpolatory quadrature rules of the highest degree of precision with preassigned nodes for general weight functions*, ACM Trans. Math. Software, **15** (1989b), 137–143.
- F. PEHERSTOFER, *Characterization of positive quadrature formulae*, SIAM J. Math. Anal., **12** (1981), 935–942.
- , *On the remainder of Gaussian quadrature formulas for Bernstein-Szegő weight functions*, Math. Comp., **60** (1993), 317–325.
- I. G. PETROVSKII, *Lectures on the Theory of Integral Equations*, Grylock Press, New York, 1957.
- D. L. PHILLIPS, *A technique for the numerical solution of certain integral equations of the first kind*, J. Assoc. Computing Machinery, **9** (1962), 84–97.
- G. M. PHILLIP AND P. J. TAYLOR, *Theory and Applications of Numerical Analysis*, 2nd ed., Academic Press, London, 1996.
- J. L. PHILLIPS, *Collocation as a projection method for solving integral and other operator equations*, Ph.D. Thesis, Purdue University, IN, 1969.
- E. PICARD, *Sur un exemple simple d'une équation singulière de Fredholm ou la nature analytique de la solution dépend au second solution*, Ann. Sci. École Norm. Sup. (3), **28** (1911), 313–324.
- R. PIESSENS, *Numerical inversion of the Laplace transform*, IEEE Trans. Automatic Control, **AC-14** (1969a), 299–301.
- , *Gaussian quadrature formulas for the numerical integration of Bromwich's integral and the inversion of the Laplace transform* (1969b), Inst. Appl. Math., University of Leuven.
- , *New quadrature formulas for the numerical inversion of the Laplace transform*, BIT, **9** (1969c), 351–361.
- , *Gaussian quadrature formulas for the numerical integration of Bromwich's integral and the inversion of the Laplace transform*, J. Engg. Math., **5** (1971a), 1–9.
- , *Calculation of Fourier coefficients of a function given at a set of arbitrary points*, Electron. Lett., **7** (1971b), 681–682.
- , *Improved method for calculation of Fourier coefficients of a function given at a set of arbitrary points*, Electron. Lett., **8** (1972a), 250–251.
- , *A new numerical method for the inversion of the Laplace transform*, J. Inst. Maths. Appl., **10** (1972b), 185–192.
- , *Algorithm 453. Gaussian quadrature formulas for Bromwich's integral*, Comm. ACM, **16** (1973a), 468–487.
- , *An algorithm for automatik integration*, Angew. Informatik, **15** (1973b), 399–401.
- , *A quadrature routine with round-off error guard*, Rep. TW 17 (1974), Appl. Math. and Prog. Div., Kath. Univ. Leuven.
- , *An automatic routine for the integration of oscillating functions*, Rep. TW 30

- (1975), *Appl. Math. and Prog. Div.*, Kath. Univ. Leuven.
- , *A bibliography on numerical inversion of Laplace transform and applications*, J. Comput. Appl. Math., **1** (1975), 115–128.
- , *A bibliography on numerical inversion of Laplace transform and applications: A supplement*, J. Comput. Appl. Math., **2** (1976), 225–228.
- , *Automatic computation of Bessel function integrals*, Comp. Phys. Comm., **25** (1982a), 289–295.
- , *Algorithm 113: Inversion of the Laplace transform*, Algorithm Supplement, Computer J., **25** (1982b), 278–282.
- , *An algorithm for a special case of a generalization of the Richardson extrapolation process*, Numer. Math., **38** (1982), 299–307.
- , *Modified Clenshaw-Curtis integration and applications to numerical computation of integral transforms*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 35–51.
- , *On rates of acceleration of extrapolation methods for oscillatory infinite integrals*, BIT, **30** (1990), 347–357.
- AND M. BRANDERS, *Numerical inversion of the Laplace transform using generalized Laguerre polynomials*, Proc. IEEE, **118** (1971), 1517–1522.
- AND M. BRANDERS, *The evaluation and application of some modified moments*, BIT, **13** (1973), 443–450.
- AND M. BRANDERS, *A note on the optimal addition of abscissas to quadrature formulas of Gauss and Lobatto type*, Math. Comp., **28** (1974), 135–140; 344–347.
- AND M. BRANDERS, *Computation of oscillatory integrals*, J. Comput. Appl. Math., **1** (1975), 153–164.
- AND M. BRANDERS, *Algorithm 002. Computation of oscillating integrals*, J. Comput. Appl. Math., **1** (1975), 153–164.
- AND M. BRANDERS, *Tables of Gaussian Quadrature Formulas*, Academic Press, Leuven, 1975.
- AND M. BRANDERS, *Computation of oscillating integrals*, J. Comp. Appl. Math., **1** (1975), 153–.
- AND M. BRANDERS, *Modified Clenshaw-Curtis method for the computation of Bessel function integrals*, BIT, **23** (1983), 370–381.
- AND M. BRANDERS, *Computation of Fourier and Laplace transforms of singular functions using modified moments*, Comp. Math. Appls., **12B** (1986), 1241–1248.
- , E. DE DONCKER-KAPENGA, C. W. ÜBERHUBER, AND D. K. KAHANER, *QUADPACK — A Subroutine Package for Automatic Integration*, Springer-Verlag, Berlin, 1983.
- , E. DE DONCKER-KAPENGA, C. W. ÜBERHUBER, AND M. D. K. KAHANER, *QUADPACK, A Quadrature Subroutine Package*, Series in Computational Math., vol. 1, Springer-Verlag, Berlin, 1983.
- AND A. HAEGEMANS, *Numerical evaluation of Fourier transform integrals*, Electron Lett., **9** (1973), 108–109.
- AND A. HAEGEMANS, *Algorithm 22. Automatic integration of highly oscillatory functions*, Computing, **13** (1974), 183–193.
- AND R. HUYSMANS, *Algorithm 619: Automatic numerical inversion of Laplace transform*, ACM Trans. Math. Software, **10** (1984), ?.
- , I. MERTENS AND M. BRANDERS, *Automatic integration of functions having algebraic end point singularities*, Angewandte Informatik, **2** (1974), 65–68.
- AND F. POLEUNIS, *A numerical method for the integration of oscillatory functions*, BIT, **11** (1971), 317–327.
- , VAN ROY-BRANDERS AND I. MERTENS, *Automatic evaluation of Cauchy principal value integrals*, Angewandte Informatik, **18** (1976), 31–35.
- AND P. VERBAETEN, *Numerical solution of the Abel integral equation*, Nordisk Tid-

- skr. Informationsbehandlung (BIT), **13** (1973), 451–457.
- J. C. PIQUETTE, *A method for symbolic evaluation of infinite integrals containing special functions or their products*, J. Symbolic Comput., **11** (1991), 231–249.
- E. POINCARÉ, *Remarque diverses sur l'équation de Fredholm*, Acta Math., **33** (1910), 57–89.
- H. POLLARD, *Note on the inversion of the Laplace integral*, Dume Math. J., **6** (1940), 420–424.
- G. POLYA, *Über Konvergenz von Quadraturverfahren*, Math. Zeit., **37** (1933), 264–286.
- A. D. POLYANIN AND A. V. MANZHIROV, *Handbook of Integral Equations*, CRC Press, Boca Raton, FL, 1998.
- D. PORTER AND D. S. G. STIRLING, *Integral Equations*, Cambridge University Press, Cambridge, 1993.
- E. L. POST, *Generalized Differentiation*, Trans. Amer. Math. Soc., **32** (1930), 723–793.
- M. J. D. POWELL, *On best L_2 spline approximations*, in Numerische Mathematik, Differentialgleichungen, Approximationstheorie, Birkhäuser, Basel, 1968, pp. 317–336.
- , *Approximation Theory and Methods*, Cambridge Univ. Press, Cambridge, 1981.
- W. H. PRESS, B. P. FLANNERY, S. A. TEUKOLSKY, AND W. T. VETTERLING, *Numerical Recipes*, Cambridge University Press, London, 1986.
- , *Numerical Recipes in Fortran*, Cambridge University Press, New York, 1992.
- J. F. PRICE, *Discussion of quadrature formulas for use on digital computers*, Rep. D1-82-0052, Boeing Sci. Res. Labs. (1960).
- P. PURI, *Impulsive motion of a flat plate in a Rivlin-Ericksen fluid*, Rheol. Acta, **23** (1984), 451–453.
- AND P. K. KULSHRESTHA, *Rotating flow of non-Newtonian fluids*, Applicable Anal., **4** (1974), 131–140.
- AND P. K. KULSHRESTHA, *Unsteady hydromagnetic boundary layer in a rotating medium*, Trans. ASME, J. Appl. Mech., **98** (1976), 205–208.
- AND P. K. KYTHE, *Some inverse Laplace transforms of exponential form*, ZAMP, **39** (1988), 150–156.
- P. RABINOWITZ, *Abscisses and weights for Lobatto quadrature of high order*, Math. Comp., **14** (1960), 47–52.
- , *Rates of convergence of Gauss, Lobatto, and Radau integration rules for singular integrands*, Math. Comp., **41** (1983), 63–78.
- , *Gauss-Kronrod integration rules for Cauchy principal value integrals*, Math. Comp., **41** (1983), 63–78.
- , *The convergence of noninterpolatory product integration rules*, BIT, **26** (1986), 131–134.
- , *Numerical integration in the presence of an interior singularity*, J. Comp. Appl. Math., **17** (1987), 31–41.
- , *Convergence results for piecewise linear quadratures for Cauchy principal value integrals*, Math. Comp., **51** (1988), 741–747.
- , *On an interpolatory product rule for evaluating Cauchy principal value integrals*, BIT, **29** (1989), 347–355.
- , *Generalized noninterpolatory rules for Cauchy principal value integrals*, Math. Comp., **54** (1990), 271–279.
- , *Numerical evaluation of Cauchy principal value integrals with singular integrands*, Math. Comp., **55** (1990), 265–270.
- , *Product integration of singular integrands using Hermite-Fejér interpolation*, BIT, **31** (1991), 321–327.
- , *Uniform convergence results for Cauchy principal value integrals*, Math. Comp., **56** (1991), 731–740.
- , *Application of approximating splines for the solution of Cauchy singular integral equations*, Trans. Appl. Numer. Math., **15** (1994), 285.
- AND N. RICHTER, *Perfectly symmetric two-dimensional integration formulas with*

- minimal number of points*, Math. Comp., **23** (1969), 765–799.
- , *The convergence of interpolatory product integration rules*, BIT, **26** (1986), 131–134.
- , *Numerical integration in the presence of an interior singularity*, J. Comp. Appl. Math., **17** (1987), 31–41.
- , *The convergence of noninterpolatory product integration rules*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 1–16.
- , *Numerical integration based on approximating splines*, J. Comput. Appl. Math., **33** (1990), 73–83.
- , *Application of approximating splines for the solution of Cauchy singular integral equations*, Trans. Appl. Numer. Math., **15** (1994), 285.
- , J. KAUTSKY, S. ELHAY, AND J. C. BUTCHER, *On sequences of imbedded integration rules*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 113–139.
- AND D. S. LUBINSKY, *Noninterpolating integration rules for Cauchy principal value integrals*, Math. Comp., **53** (1989), 279–295.
- AND E. SANTI, *On the uniform convergence of Cauchy principal values of quasi-interpolating splines*, BIT, **35** (1995), 277–290.
- AND I. H. SLOAN, *Product integration in the presence of a singularity*, SIAM J. Numer. Anal., **21** (1984), 149–166.
- AND W. E. SMITH, *Interpolatory product integration in the presence of singularities: L_2 theory*, J. Comput. Appl. Math., **39** (1992), 79–87.
- AND W. E. SMITH, *Interpolatory product integration in the presence of singularities: L_p theory*, in Numerical Integration — Recent Developments, Software and Applications (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 93–109.
- R. RADAU, *Étude sur les formules d'approximation qui servent à calculer la valeur numérique d'une intégrale définie*, J. Math. Pures Appl., (3), **6** (1880), 283–336.
- E. D. RAINEVILLE, *Special Functions*, Macmillan & Co., New York, 1960.
- A. RALSTON, *A family of quadratures which achieve high accuracy in composite rules*, J. ACM, **6** (1959), 384–394.
- AND P. RABINOWITZ, *A First Course in Numerical Analysis*, 2nd ed., McGraw-Hill, New York, 1978.
- L. REISCHEL, *Parallel iterative methods for the solution of Fredholm integral equations of the second kind*, in Hypercube Multiprocessors (M. T. Heath, ed.), SIAM, Philadelphia, PA, 1987, pp. 520–529.
- , *Fast solution methods for Fredholm integral equations of the second kind*, Numer. Math., **57** (1989), 719–736.
- J. R. RICE (ed.), *Mathematical Software*, Academic Press, New York, 1971.
- , *A metaalgorithm for adaptive quadrature*, J. ACM, **22** (1975), 61–82.
- , *Numerical Methods, Software, and Analysis*, McGraw-Hill, New York, 1983.
- J. F. RITT, *Integration in Finite Terms*, Columbia Univ. Press, New York, 1948.
- T. J. RIVLIN, *An Introduction to the Approximation of Functions*, Dover, New York, 1981.
- , *The Chebyshev Polynomials*, 2nd ed., Wiley, New York, 1990.
- M. RIZZARDI, *A modification of Talbot's method for the simultaneous approximation of several values of the inverse Laplace transform*, ACM Trans. Math. Software, **21** (1995), 347–371.
- F. J. RIZZO AND D. J. SHIPPY, *A method of solution for certain problems of transient heat conduction*, AIAA J., **8** (1970), 2004–2009.
- G. E. ROBERTS AND H. KAUFMAN, *Table of Laplace Transform*, W. B. Saunders Company, Philadelphia and London, 1966.
- I. G. ROBINSON, *Adaptive Gaussian integration*, Austral. Comput. J., **3** (1971), 126–129.

- AND E. DE DONCKER, *Algorithm 45. Automatic computation of improper integrals over a bounded or unbounded planar region*, Computing, **25** (1981), 253–284.
- G. RODRIGUEZ AND S. SEATZU, *On the numerical inversion of the Laplace transform in reproducing kernel Hilbert spaces*, IMA J. Numer. Anal., **13** (1993), 463–475.
- C. J. ROTHART AND H. FIOLET, *Quadrature procedures*, Report MR 137/72 (1972), Mathematisch Centrum, Amsterdam.
- M. ROSENLICHT, *Integration in finite terms*, Amer. Math. Monthly, **79** (1972), 963–972.
- H. RUTISHAUSER, *Ausdehnung des Romberg'schen Prinzips*, Num. Math., **5** (1963), 48–54.
- , *On a modification of the QD-algorithm with Graeffe-type convergence*, in Proc. IFIP Congress 62, North-Holland, Amsterdam, 1993.
- A. SAENGER, *On a numerical quadrature of Fourier transform*, J. Math. Anal. Appl., **8** (1964), 1–3.
- S. SAITOH, *One approach to some general integral transforms and its applications*, Integral Eqs. and Special Functions, **3** (1995), 49–84.
- H. E. SALZER, *Orthogonal polynomials arising in the numerical evaluation of inverse Laplace transform*, Mathematical Tables and Other Aids to Computation, **9** (1955), 163–177.
- , *Equally weighted quadrature formulas over semi-infinite and infinite intervals*, J. Math. Phys., **34** (1955), 54–63.
- , *Tables for the numerical calculation of inverse Laplace transforms*, J. Math. Phys., **37** (1958), 89–108.
- , *Additional formulas and tables for orthogonal polynomials originating from inversion integrals*, J. Math. Phys., **40** (1961), 72–86.
- G. SANSONE, *Functional Analysis*, McGraw-Hill, New York, 1973.
- J. SARANEN AND I. H. SLOAN, *Quadrature methods for logarithmic-kernel integral equations on closed curves*, IMA J. Numer. Anal., **12** (1992), 167.
- A. SARD, *Integral representations of remainders*, Duke Math. J., **15** (1948), 333–345.
- , *Best approximate integration formulas; best approximation formulas*, Amer. J. Math., **71** (1949), 80–91.
- AND L. F. MEYERS, *Best approximate integration formulas*, J. Math. Phys., **29** (1950), 118–123.
- , *Linear Approximation*, American Math. Soc., Providence, RI, 1963.
- R. A. SCHAPERY, *Approximate methods of transform inversion for viscoelastic stress analysis*, Proc. Fourth U.S. National Congr. Appl. Mech. (1961), 1075–1085.
- , *Approximate methods of transform inversion for viscoelastic stress analysis*, Proc. 4th U.S. Nat. Congr. Appl. Mech., ASME, **2** (1962), 1075–1085.
- F. SCHEID, *Theory and Problems of Numerical Analysis*, Schaum's Outline Series, McGraw-Hill, New York, 1968.
- T. SCHIRA, *The remainder term for analytic functions of Gauss-Lobatto quadratures*, J. Comp. Appl. Math., **76** (1996), 171–193.
- , *The remainder term for analytic functions of symmetric Gaussian quadratures*, Math. Comp., **66** (1997), 297–310.
- G. SCHMEISSER AND H. SCHIRMEIER, *Praktische Mathematik*, Walter de Gruyter, Berlin, 1976.
- L. A. SCHMITTROTH, *Numerical inversion of Laplace transforms*, Comm. ACM, **3** (1960), 171–173.
- C. SCHNEIDER, *Regularity of the solution to a class of weakly singular Fredholm integral equations of the second kind*, Integral Eqs. Operator Theory, **2** (1979), 62–68.
- , *Product integration for weakly singular integral equations*, Math. Comput., **36** (1981a), 207–213.
- , *Produktintegration zur Lösung schwachsingulären Integralgleichungen*, ZAMM, **8** (1981b), T317–319.
- L. A. SCHMITTROTH, *Numerical inversion of Laplace transforms*, Comm. ACM, **3** (1960),

171–173.

- C. SCHWARTZ, *Numerical evaluation of analytic functions*, J. Comp. Phys., **4** (1969), 19–29.
- T. S. SHAO, T. C. CHEN, AND R. M. FRANK, *Tables of zeros and Gaussian weights of certain associated Laguerre polynomials and the related generalized Hermite polynomials*, Math. Comp., **18** (1964), 598–616.
- L. F. SHAMPINE AND R. C. ALLEN, JR., *Numerical Computing: An Introduction*, W. B. Saunders, Philadelphia, Pa, 1973.
- D. SHANKS, *Non-linear transformations of divergent and slowly convergent sequences*, J. Math. Phys., **34** (1955), 1–42.
- C. E. SHANNON, *Communications in the presence of noise*, Proc. Inst. Radio Eng., **37** (1949), 10–21.
- B. G. SHERLOCK AND D. M. MONRO, *Algorithm 749: Fast discrete cosine transform*, ACM Trans. Math. Software, **21** (1995), 372–378.
- J. SHOAT, *Laguerre polynomials and the Laplace transform*, Duke Math. J., **6** (1940), 615–626.
- A. SIDI, *Some properties of a generalization of the Richardson extrapolation process*, J. Inst. Math. Appl., **24** (1979), 327–346.
- , *Extrapolation methods for oscillatory infinite integrals*, J. Inst. Math. Appl., **26** (1980), 1–20.
- , *The numerical evaluation of very oscillatory infinite integrals by extrapolation*, Math. Comp., **38** (1982), 517–529.
- , *An algorithm for the special case of a generalization of the Richardson extrapolation process*, Numer. Math., **38** (1982), 299–307.
- , *The numerical evaluation of very oscillatory infinite integrals by extrapolation*, Math. Comp., **38** (1982), 517–529.
- , *Extrapolation methods for divergent oscillatory infinite integrals that are defined in the sense of summability*, J. Comp. Appl. Math., **17** (1987), 105–114.
- , *Generalizations of Richardson extrapolation with applications to numerical integration*, in Numerical Integration III— Proceedings of the Conference at the Mat. Inst., Oberwolfach, 1988 (H. Braß and G. Hämmerlin, eds.), Birkhäuser, Basel, 1988, pp. 237–250.
- , *A user-friendly extrapolation method for infinite integrals*, Math. Comp., **51** (1988), 249–266.
- , *Comparison of some numerical quadrature formulas for weakly singular periodic Fredholm integral equations*, Computing: Archiv für Informatik und Numerik., **43** (1989), 159.
- , *On rates of acceleration of extrapolation methods for oscillatory infinite integrals*, BIT, **30** (1990), 347–357.
- , *Computation of oscillatory infinite integrals by extrapolation methods*, in Numerical Integration — Recent Developments, Software and Applications (T. O. Espelid and A. Genz, eds.), Kluwer, Dordrecht, 1992, pp. 349–351.
- , *A new variable transformation for numerical integration*, in Numerical Integration III — Proceedings of the Conference at the Mat. Inst., Oberwolfach, 1992 (H. Braß and G. Hämmerlin, eds.), Birkhäuser, Basel, 1993, pp. 359–373.
- P. SILVESTER, *Symmetric quadrature formulae for simplexes*, Math. Comput., **24** (1970), 95–100.
- R. C. SINGLETON, *On computing the fast Fourier transform*, Comm. ACM, **10** (1967), 647–654.
- N. S. SKOBYLA, *Tables for the Numerical Inversion of the Laplace Transforms*, Izdat. Akad. Nauk BSSR, Minsk, 1964. (Russian)
- I. H. SLOAN, *Iterated Galerkin method for eigenvalue problems*, SIAM J. Numer. Anal., **13** (1976), 753–760.
- , *On the numerical evaluation of singular integrals*, BIT, **18** (1978), 91–102.

- , *The numerical solution of Fredholm equations of the second kind by polynomial interpolation*, Technical Note BN 905 (1979), University of Maryland.
- , *On choosing the points in product integration*, J. Phys. Phys., **21** (1980), 1032–1039.
- , *The numerical solution of Fredholm equations of the second kind*, J. Integral Eq., **2** (1980), 265–279.
- , *A review of numerical methods for Fredholm equations of the second kind*, in The Application and Numerical Solution of Integral Equations (R. S. Anderssen, F. R. de Hoog and M. A. Lukas, eds.), Sijthoff and Noordhoff, Alphen aan den Rijn, 1980.
- , B. BURN, AND N. DATYNER, *A new approach to the numerical solution of integral equations*, J. Comput. Phys., **18** (1975).
- AND B. BURN, *Collocation with polynomials for integral equations of the second kind: A new approach to the theory*, J. Integral Eq., **1** (1979), 77–94.
- AND W. E. SMITH, *Product-integration with the Clenshaw-Curtis and related points. Convergence properties*, Numer. Math., **30** (1978), 415–428.
- AND W. E. SMITH, *Product-integration with the Clenshaw-Curtis and related points. Implementation and error estimates*, Numer. Math., **34** (1980), 387–401.
- AND W. E. SMITH, *Properties of interpolatory product integration rules*, SIAM J. Numer. Anal., **19** (1982), 427–442.
- B. T. SMITH, J. M. BOYLA, B. S. GARBOW, Y. IKEBE, V. C. KLEMA, AND C. B. MOLER, *Matrix Eigensystem Routines — EISPACK Guide*, Lecture Notes in Computer Science #6, 2nd ed., Springer-Verlag, Berlin, 1976.
- F. J. SMITH, *Quadrature methods based on the Euler-Maclaurin formula and on the Clenshaw-Curtis method of integration*, Numer. Math., **7** (1965), 406–411.
- W. E. SMITH AND I. H. SLOAN, *Product integration rules based on the zeros of Jacobi polynomials*, SIAM J. Numer. Anal., **17** (1980), 1–13.
- I. H. SLOAN, AND A. H. OPIE, *Product integration over infinite intervals. I. Rules based on the zeros of Hermite polynomials*, Math. Comp., **40** (1983), 519–535.
- AND D. F. PAGET, *Optimal nodes for interpolatory product integration*, SIAM J. Numer. Anal., **29** (1992), 586–600.
- I. N. SNEDDON, *Fourier Transform and Its Applications*, Springer-Verlag, Berlin, 1978.
- A. SPENCE, *Product integration for singular integrals and singular integral equations*, in Numerische Integration (G. Hämmerlin, eds.), ISNM 45, Birkhäuser, Basel, 1979.
- M. R. SPIEGEL, *Mathematical Handbook of Formulas and Tables*, McGraw-Hill, New York, 1968.
- W. SQUIRE, *Comment on numerical calculation of Fourier transform integrals*, Electron. Lett. Math., **9** (1973), 291.
- , *Partition-extrapolation methods for numerical quadrature*, Intern. J. Comput. Math., **5** (1975), 81–91.
- , *A quadrature method for finite intervals*, Intern. J. Numer. Methods in Engg., **10** (1976a), 708–712.
- , *Integration for Engineers and Scientists*, Amer. Elsevier, New York, 1976b.
- , *A comment on quadrature in the presence of end-point singularities*, Int. J. Comp. Math., **7** (1979), 239–241.
- , *Comparison of Gauss-Hermite and midpoint quadrature with application to the Voigt function*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 111–112.
- H. STEHFEST, *Algorithm 368: Numerical inversion of Laplace transform*, Comm. ACM, **13** (1970a), 47–49.
- , *Remark on Algorithm 368*, Comm. ACM, **13** (1970b), 624.
- E. M. STEIN AND G. WEISS, *Introduction to Fourier Analysis on Euclidean Spaces*, Princeton Univ. Press, NJ, 1971.

- T. J. STIELTJES, *Quelques recherches sur la theorie des quadratures dites mécanique*, Ann. Sci. École Norm. Sup., (3), **1** (1884), 409–426.
- M. R. SPIEGEL, *Mathematical Handbook of Formulas and Tables*, Schaum's Outline Series, McGraw-Hill, New York, 1968.
- P. STIGALL, R. E. ZIEMER AND L. HUDEC, *A performance study of 16-bit microcomputer-implemented FFT algorithms*, IEEE Micro, (1982), 61.
- U. STORCK, *Verified calculation of the nodes and weights for Gaussian quadrature formulas*, Interval Compu., **4** (1993), 114–124.
- J. O. STRÖMBERG, *A modified Franklin system and higher order spline systems on R^n as unconditional basis for Hardy spaces*, in Conference in Honor of A. Zygmund (W. Beckner, ed.), Vol. II, Wadsworth, 1981, pp. 475–493.
- A. H. STROUD, *Approximate Calculation of Multiple Integrals*, Prentice-Hall, Englewood Cliffs, NJ, 1971.
- , *Numerical Quadrature and Solution of Ordinary Differential Equations*, Springer-Verlag, New York, 1974.
- and D. SECREST, *Gaussian Quadrature Formulas*, Prentice-Hall, Englewood Cliffs, NJ, 1966.
- , *Interactive numerical quadrature*, in Numerical Integration — Recent Developments, Software and Applications (P. Keast and G. Fairweather, eds.), D. Reidel, Dordrecht, the Netherlands, 1987, pp. 291–306.
- F. STUMMEL AND K. HAINER, *Praktische Mathematik*, 2nd. ed., Teubner, Stuttgart, 1982.
- M. SUGIHARA, *Methods of numerical integration of oscillatory functions by the DE-formula with Richardson extrapolation*, J. Comp. Appl. Math., **17** (1987a), 47–68.
- G. T. SYMM, *Integral equation methods in potential theory, II*, Proc Royal Soc., Ser. A **275** (1963), 33–46 (for part I, see M. A. Jawson).
- , *An integral equation method in conformal mapping*, Numerische Math. **9** (1966), 250–258.
- , *Problems in two-dimensional potential theory (Ch. 20). Potential problems in three dimensions (Ch. 24)*, in Numerical Solution of Integral Equations (L. M. Delves and J. Walsh, eds.), Clarendon Press, Oxford, 1974, pp. 267–274; 312–320.
- G. SZEGÖ, *Orthogonal Polynomials*, Colloquium Publications, # 23, Amer. Math. Soc., 1939.
- H. TAKAHASI AND M. MORI, *Estimation of errors in the numerical quadrature of analytic functions*, Applicable Anal., **1** (1971), 201–229.
- AND M. MORI, *Quadrature formulas obtained by variable transformation*, Numer. Math., **21** (1973), 206–219.
- A. TALBOT, *The accurate numerical inversion of Laplace transforms*, J. Inst. Maths. Applics., **23** (1979), 97–120.
- R. I. TANNER, *An inversion formula for the Laplace integral*, Duke Math. J., **6** (1940), 1–26.
- C. TASWELL AND K. C. MCGILL, *Algorithm 735: Wavelet transform algorithms for finite-duration discrete-time signals*, ACM Trans. Math. Software, **20** (1994), 398–426.
- H. J. J. TE RIELE, *A program for solving the first kind Fredholm integral equations by means of regularisation*, Report NM-R8416, Dept. of Numerical Math., Amsterdam (1984).
- D. TER HAAR, *An easy approximate method of determining the spectrum of a viscoelastic material*, J. Polymer Sci., **6** (1951), 247.
- THE MATHWORKS, *MATLAB*, Version 6, The MathWorks, Natick, MA, 1984–2000.
- P. S. THEOCARIS AND N. I. IOAKIMIDIS, *On the numerical solution of Cauchy type singular integral equations and the determination of stress intensity factors in case of complex singularities*, ZAMM, **28** (1977), 1085–1098.
- A. N. TIKHONOV, *On the solution of ill-posed problems and the method of regularization*, Soviet Math. Dokl., **4** (1963), 1035–1038.
- AND V. B. GLASKO, *An approximate solution of Fredholm integral equation of the*

- first kind*, Zhurnal vychislitel'noy matematiki i matematicheskoy Fiziki, **4** (1964), 564–571 (Russian).
- S. TIMOSHENKO AND J. N. GOODIER, *Mathematical Theory of Elasticity*, McGraw-Hill, New York, 1951.
- H. TODA AND H. ONO, *Notes on effective usage of double exponential formulas for numerical integration*, in *Numerical Integration and Related Topics* (M. Mori, eds.), RIMS Kokyuroka 401, Kyoto Univ., 1980, pp. 21–47.
- J. N. TOKIS, *Unsteady magnetohydrodynamic free-convection flows in a rotating fluid*, Astrophys. Space Sc., **119** (1996), 305–313.
- H.-J. TÖPLER AND W. VOLK, *Die numerische Behandlung von Integralgleichungen zweiten Art mittels Splinefunktionen*, in *Numerical Treatment of Integral Equations* (J. Albrecht and L. Collatz, eds.), ISNM 53, Birkhäuser, Basel, 1980, pp. 228–243.
- L. N. TREFETHEN (ed.), *Numerical Conformal Mapping*, North-Holland, Amsterdam, 1986.
- F. G. TRICOMI, *Integral Equations*, Wiley Interscience, New York, 1957.
- A. N. TIKHONOV, *On the solution of ill-posed problems and the method of regularization*, Soviet Math. Dokl., **4** (1963), 1035–1038.
- AND V. B. GLASKO, *An approximate solution of Fredholm integral equation of the first kind*, Zhurnal vychislitel'noy matematiki i matematicheskoy Fiziki, **4** (1964), 564–571 (Russian).
- P. L. TSCHEBYSCHIEFF, *Sur les quadratures*, J. Math. Pures Appl., **19** (1874), 19–34.
- S. TWOMEY, *On the numerical solution of Fredholm integral equations of the first kind by the inversion of the linear system produced by quadrature*, J. Assoc. Computing Machinery, **10** (1963), 97–101.
- , *The application of numerical filtering to the solution of integral equations encountered in indirect sensing measurements*, J. Franklin Inst., **279** (1975), 95–109.
- D. Y. TZOU, *Macro to Microscale Heat Transfer: The Lagging Behaviour*, Taylor and Francis, Washington, 1997.
- , M. N. ÖZISIK, AND R. J. CHIFFELLE, *The lattice temperature in the microscopic two-step model*, J. Heat Transfer, Trans. ASME, **116** (1994), 1034–1038.
- AND Y. S. ZHANG, *An analytical study of the fast-transient process in small scales*, Int. J. Eng. Sci., **33** (1995), 1449–1463.
- J. L. ULLMAN, *A class of weight functions that admit Tschebyscheff quadrature*, Michigan Math. J., **13** (1966), 417–423.
- G. M. VAINIKKO AND A. PEDAS, *The properties of solutions of weakly singular integral equations*, J. Aust. Math. Soc., Ser. B, **22** (1981), 419–430.
- AND P. UBAS, *A piecewise polynomial approximation to the solution of an integral equation with weakly singular kernel*, J. Aust. Math. Soc., Ser. B, **22** (1981), 431–438.
- J. M. VARAH, *Pitfalls in the numerical solution of linear ill-posed problems*, SIAM J. Sci. Statist. Comput. **4** (1983), 164–176.
- N. P. VEKUA, *Systems of Singular Integral Equations*, P. Noordhoff, The Netherlands, 1967.
- P. VÉRTESI, *Remarks on convergence of Gaussian quadrature for singular integrals*, Acta Math. Hung., **53** (1989), 399–405.
- T. VON PETERSDORFF, C. SCHWAB, AND R. SCHNEIDER, *Multiwavelets for second kind integral equations*, SIAM J. Numer. Anal., **34** (1997), 2212.
- G. WAHBA, *Practical approximate solutions of linear operator equations when the data are noisy*, SIAM J. Appl. Math. **14** (1977), 651–667.
- G. C. WALLICK, *Remark on algorithm 351. Modified Romberg quadrature*, ZAMM, **53** (1973), 1–8.
- J. S. WALKER, *Fast Fourier Transforms*, CRC Press, Boca Raton, FL, 1991.
- G. G. WALTER, *Wavelets and Other Orthogonal Systems with Applications*, CRC Press, Boca Raton, FL, 1994.
- , *Pointwise convergence for wavelet expansions*, J. Approx. Theory, **80** (1995), 108–118.

- W. T. WEEKS, *Numerical inversion of Laplace transforms*, J. ACM, **13** (1966), 419–426.
- J. A. C. WEIDEMAN, *Algorithms for parameter selection in the Weeks method for inverting Laplace transforms*, SIAM J. Sci. Comput., **21** (1999), 111–128.
- B. WENDROFF, *Theoretical Numerical Analysis*, Academic Press, New York, 1966.
- H. WERNER AND D. ZWICK, *Algorithms for numerical integration with regular splines*, Report No. 27 (1977), Rechenzentrum der Universität Münster.
- A. D. WHEELON, *Tables of Summable Series and Integrals Involving Bessel Functions*, Holden-Day, San Francisco, 1968.
- V. WICKERHAUSER, *Adapted Wavelet Analysis from Theory to Software*, AK Peters, Boston, 1994.
- D. V. WIDDER, *The inversion of the Laplace transform and the related moment problem*, Trans. Amer. Math. Soc., **36** (1934), 107–200.
- , *An application of Laguerre polynomials*, Duke Math. J., **1** (1935), 126–136.
- H. S. WILF, *The possibility of Tschebyscheff quadrature on infinite intervals*, Proc. Nat. Acad. Sci., **47** (1961), 209–213.
- , *Exactness conditions in numerical quadrature*, Numer. Math., **6** (1964), 315–319.
- R. E. WILLIAMSON, R. H. CROWELL, AND H. F. TROTTER, *Calculus of Vector Functions*, Prentice-Hall, Englewood Cliffs, NJ, 1962, pp. 316.
- M. W. WILSON, *A general algorithm for nonnegative quadrature formulas*, Math. Comput., **23** (1969), 253–258.
- J. WIMP, *Computation with Recurrence Relations*, Pitman Press, 1984.
- G. M. WING, *A Primer on Integral Equations of the First Kind*, SIAM, Philadelphia, 1991.
- O. WING, *An efficient method of numerical inversion of Laplace transform*, Computing, **2** (1967), 153–166.
- P. WOJTAŚCZYK, *The Franklin system is an unconditional basis in H^1* , Archiv für Mat., **20** (1982), 293–300.
- K. B. WOLF, *Integral Transforms in Science and Engineering*, Plenum Press, New York, 1979.
- S. WOLFRAM, *Mathematica*, 2nd ed., Addison-Wesley, New York, 1991.
- , *The Mathematica Book*, 3rd ed., Wolfram Media, Champaign, IL, and Cambridge University Press, Cambridge, UK, 1996.
- P. WYNN, *On a device for computing the $e_m(S_n)$ transformation*, Math. Comp., **10** (1956), 91–96.
- Y. XU, *Common Zeros of Polynomials in Several Variables and Higher Dimension Quadrature*, Pitman Series, Longman Scientific And Tech., 1994.
- Y. YAN, *A fast numerical solution for a second kind integral equations with a logarithmic kernel*, SIAM J. Numer. Math., **31** (1994), 477–498.
- A. YOUNG, *Approximate product-integration*, Proc. Roy. Soc. London, Ser. A, **224** (1954a), 552–561.
- , *The application of approximate product-integration to the numerical solution of integral equations*, Proc. Roy. Soc. London, Ser. A, **224** (1954b), 561–573.
- S. WOLFRAM, *The Mathematica Book*, 4th Ed., Wolfram Media/Cambridge University Press, New York, 1999.
- A. ZYGMUND, *Trigonometric Series*, Cambridge Univ. Press, New York, 1957.